



Full wwPDB EM Validation Report ⓘ

Dec 2, 2025 – 01:42 AM JST

PDB ID : 9L15 / pdb_00009l15
EMDB ID : EMD-62734
Title : Structure of SARS-CoV-2 EG.5.1 Variant Spike protein complexed with anti-body XGi-203
Authors : Qiu, Y.N.; Sun, L.
Deposited on : 2024-12-13
Resolution : 2.95 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

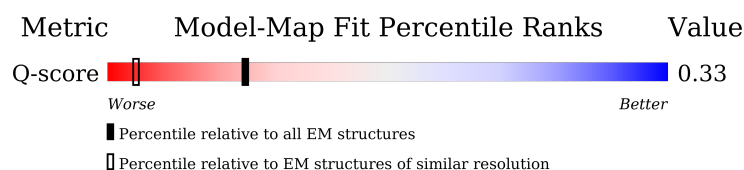
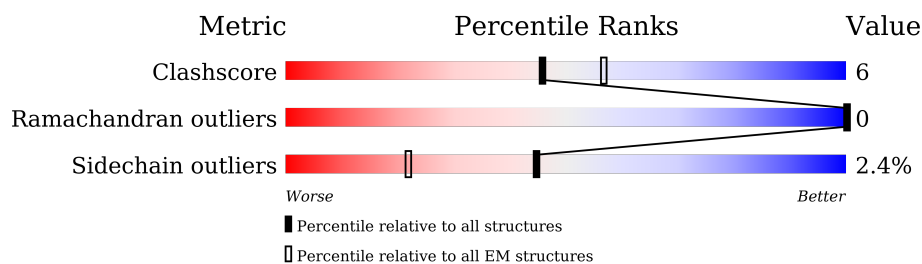
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13114 (2.45 - 3.45)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	453	
1	I	453	
1	J	453	
2	L	217	


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Mol	Chain	Length	Quality of chain
2	M	217	
2	N	217	
3	A	1295	
3	B	1295	
3	C	1295	
4	D	2	
4	E	2	
4	G	2	
4	K	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	
4	c	2	
4	d	2	

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Mol	Chain	Length	Quality of chain
5	F	3	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34509 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called XGi-203 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	214	Total	C	N	O	S	0	0
			1609	1023	270	312	4		
1	I	214	Total	C	N	O	S	0	0
			1609	1023	270	312	4		
1	J	214	Total	C	N	O	S	0	0
			1609	1023	270	312	4		

- Molecule 2 is a protein called XGi-203 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	215	Total	C	N	O	S	0	0
			1620	1006	266	342	6		
2	M	215	Total	C	N	O	S	0	0
			1620	1006	266	342	6		
2	N	215	Total	C	N	O	S	0	0
			1620	1006	266	342	6		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1019	Total	C	N	O	S	0	0
			7979	5102	1327	1513	37		
3	B	1022	Total	C	N	O	S	0	0
			7998	5113	1333	1515	37		
3	A	1020	Total	C	N	O	S	0	0
			7980	5103	1328	1512	37		

There are 471 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	initiating methionine	UNP P0DTC2
C	-9	PRO	-	expression tag	UNP P0DTC2
C	-8	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	expression tag	UNP P0DTC2
C	-6	SER	-	expression tag	UNP P0DTC2
C	-5	LEU	-	expression tag	UNP P0DTC2
C	-4	GLN	-	expression tag	UNP P0DTC2
C	-3	PRO	-	expression tag	UNP P0DTC2
C	-2	LEU	-	expression tag	UNP P0DTC2
C	-1	ALA	-	expression tag	UNP P0DTC2
C	0	THR	-	expression tag	UNP P0DTC2
C	1	LEU	-	expression tag	UNP P0DTC2
C	2	TYR	-	expression tag	UNP P0DTC2
C	3	LEU	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	GLY	-	expression tag	UNP P0DTC2
C	6	MET	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	VAL	-	expression tag	UNP P0DTC2
C	9	ALA	-	expression tag	UNP P0DTC2
C	10	SER	-	expression tag	UNP P0DTC2
C	11	VAL	-	expression tag	UNP P0DTC2
C	12	LEU	-	expression tag	UNP P0DTC2
C	13	ALA	-	expression tag	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	52	HIS	GLN	variant	UNP P0DTC2
C	83	ALA	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	456	LEU	PHE	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2
B	-10	MET	-	initiating methionine	UNP P0DTC2
B	-9	PRO	-	expression tag	UNP P0DTC2
B	-8	MET	-	expression tag	UNP P0DTC2
B	-7	GLY	-	expression tag	UNP P0DTC2
B	-6	SER	-	expression tag	UNP P0DTC2
B	-5	LEU	-	expression tag	UNP P0DTC2
B	-4	GLN	-	expression tag	UNP P0DTC2
B	-3	PRO	-	expression tag	UNP P0DTC2
B	-2	LEU	-	expression tag	UNP P0DTC2
B	-1	ALA	-	expression tag	UNP P0DTC2
B	0	THR	-	expression tag	UNP P0DTC2
B	1	LEU	-	expression tag	UNP P0DTC2
B	2	TYR	-	expression tag	UNP P0DTC2
B	3	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	GLY	-	expression tag	UNP P0DTC2
B	6	MET	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	VAL	-	expression tag	UNP P0DTC2
B	9	ALA	-	expression tag	UNP P0DTC2
B	10	SER	-	expression tag	UNP P0DTC2
B	11	VAL	-	expression tag	UNP P0DTC2
B	12	LEU	-	expression tag	UNP P0DTC2
B	13	ALA	-	expression tag	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	52	HIS	GLN	variant	UNP P0DTC2
B	83	ALA	VAL	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	PRO	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	456	LEU	PHE	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	490	SER	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
A	-10	MET	-	initiating methionine	UNP P0DTC2
A	-9	PRO	-	expression tag	UNP P0DTC2
A	-8	MET	-	expression tag	UNP P0DTC2
A	-7	GLY	-	expression tag	UNP P0DTC2
A	-6	SER	-	expression tag	UNP P0DTC2
A	-5	LEU	-	expression tag	UNP P0DTC2
A	-4	GLN	-	expression tag	UNP P0DTC2
A	-3	PRO	-	expression tag	UNP P0DTC2
A	-2	LEU	-	expression tag	UNP P0DTC2
A	-1	ALA	-	expression tag	UNP P0DTC2
A	0	THR	-	expression tag	UNP P0DTC2
A	1	LEU	-	expression tag	UNP P0DTC2
A	2	TYR	-	expression tag	UNP P0DTC2
A	3	LEU	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	GLY	-	expression tag	UNP P0DTC2
A	6	MET	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	VAL	-	expression tag	UNP P0DTC2
A	9	ALA	-	expression tag	UNP P0DTC2
A	10	SER	-	expression tag	UNP P0DTC2
A	11	VAL	-	expression tag	UNP P0DTC2
A	12	LEU	-	expression tag	UNP P0DTC2
A	13	ALA	-	expression tag	UNP P0DTC2
A	19	ILE	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	52	HIS	GLN	variant	UNP P0DTC2
A	83	ALA	VAL	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	456	LEU	PHE	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		

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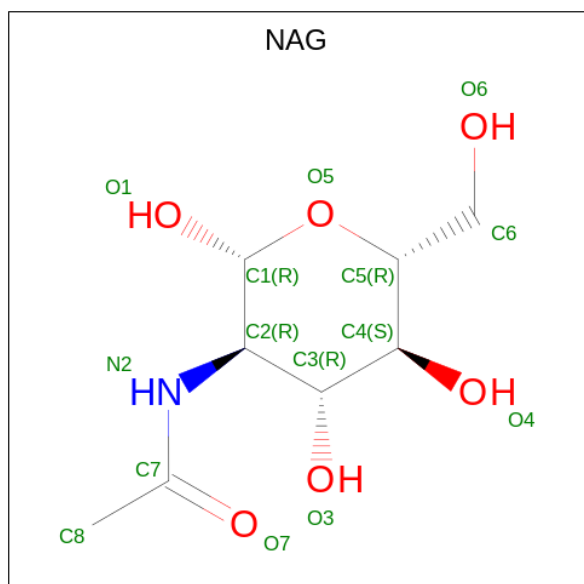
Mol	Chain	Residues	Atoms				AltConf	Trace
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	3	Total	C	N	O	0	0
			39	22	2	15		

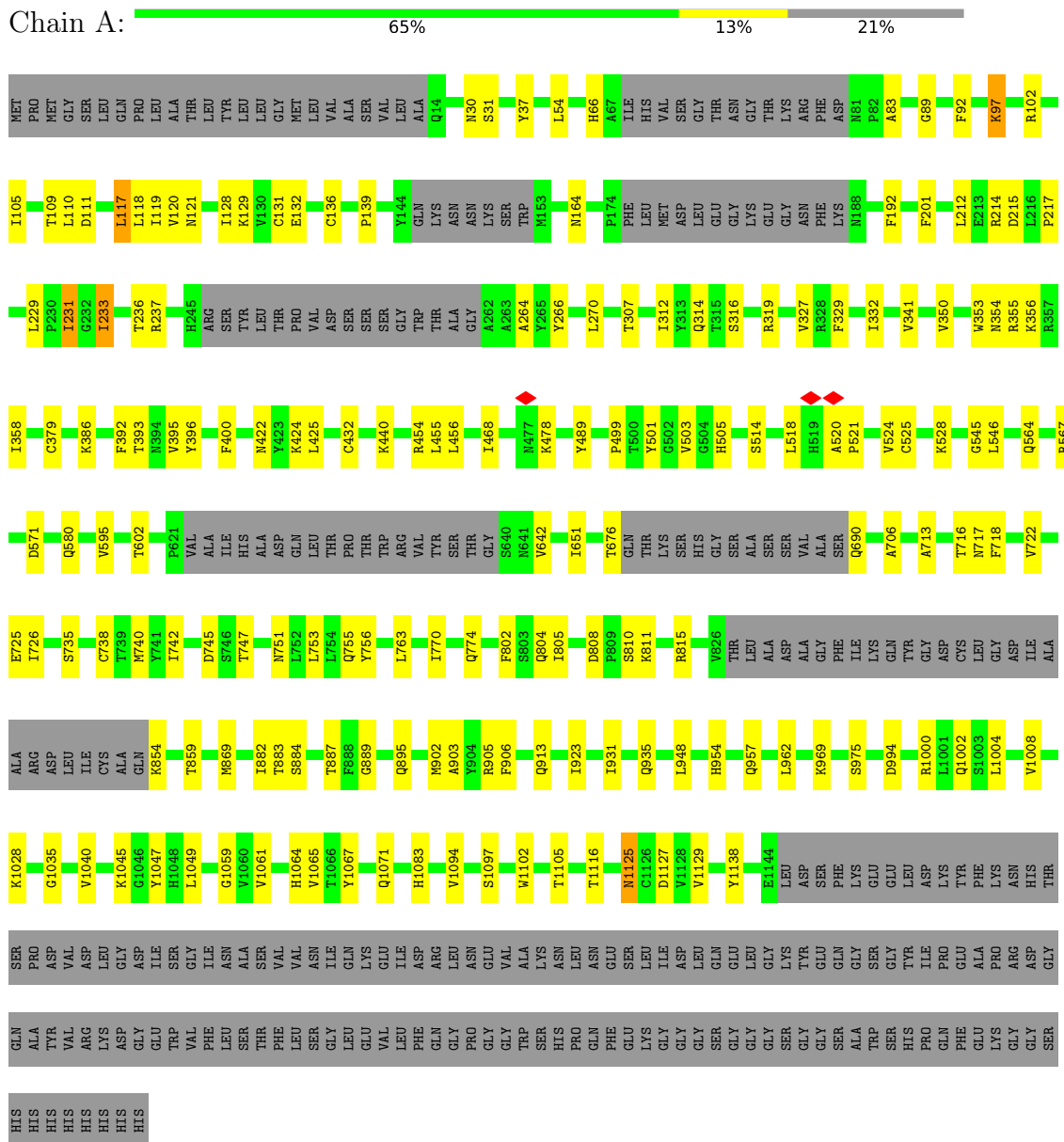
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



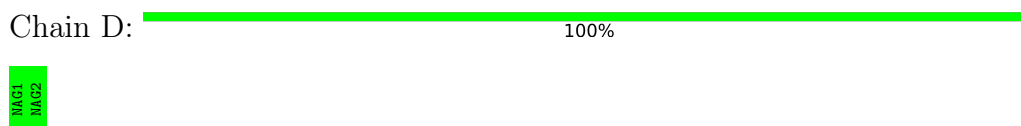
Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	



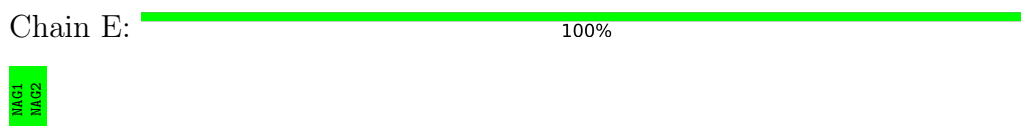




- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  50% 50%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%

MAG1
MAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32232	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.881	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	298.24, 298.24, 298.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	H	0.12	0/1650	0.37	0/2257
1	I	0.12	0/1650	0.37	0/2257
1	J	0.13	0/1650	0.34	0/2257
2	L	0.11	0/1659	0.34	0/2268
2	M	0.10	0/1659	0.34	0/2268
2	N	0.11	0/1659	0.35	0/2268
3	A	0.12	0/8169	0.32	0/11122
3	B	0.12	0/8187	0.34	0/11145
3	C	0.12	0/8167	0.33	0/11118
All	All	0.12	0/34450	0.34	0/46960

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1609	0	1585	22	0
1	I	1609	0	1585	32	0
1	J	1609	0	1585	27	0
2	L	1620	0	1537	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1620	0	1537	19	0
2	N	1620	0	1537	22	0
3	A	7980	0	7793	100	0
3	B	7998	0	7809	102	0
3	C	7979	0	7791	102	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	G	28	0	25	0	0
4	K	28	0	25	1	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	1	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	1	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
4	d	28	0	25	0	0
5	F	39	0	34	0	0
6	A	98	0	91	1	0
6	B	84	0	78	0	0
6	C	84	0	78	0	0
All	All	34509	0	33540	405	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (405) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:21:ARG:HE	3:B:80:ASP:HB3	1.41	0.85
2:M:188:GLN:HE21	2:M:194:ALA:HB2	1.50	0.75
2:N:188:GLN:HE21	2:N:194:ALA:HB2	1.56	0.71
3:A:1125:ASN:ND2	3:A:1127:ASP:OD1	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:521:PRO:HA	3:A:564:GLN:HE22	1.57	0.70
1:J:36:VAL:HG21	1:J:106:ARG:HB2	1.74	0.69
3:A:422:ASN:HD21	3:A:454:ARG:H	1.42	0.66
3:C:706:ALA:O	3:B:895:GLN:NE2	2.30	0.65
1:H:108:SER:HB2	1:H:114:THR:HB	1.78	0.64
1:J:109:VAL:HG13	1:J:112:VAL:HG22	1.81	0.63
3:B:330:PRO:HA	3:B:579:PRO:HB2	1.79	0.63
1:H:136:VAL:HG11	1:H:213:VAL:HG21	1.81	0.63
3:B:106:PHE:HB2	3:B:117:LEU:HB3	1.81	0.63
2:M:94:LEU:HD21	2:M:124:LEU:HD21	1.81	0.62
3:A:811:LYS:NZ	3:A:815:ARG:O	2.32	0.62
3:C:393:THR:HG21	3:C:519:HIS:HB3	1.82	0.62
2:L:155:CYS:HB3	2:L:197:SER:HB3	1.81	0.61
3:A:1047:TYR:HB2	3:A:1067:TYR:HB3	1.83	0.61
3:A:804:GLN:OE1	3:A:935:GLN:NE2	2.34	0.60
3:B:87:ASN:ND2	3:B:88:ASP:OD1	2.34	0.60
3:B:763:LEU:HD22	3:B:1008:VAL:HG21	1.83	0.60
3:B:1116:THR:HG22	3:B:1138:TYR:HB3	1.83	0.60
3:C:383:SER:HB3	3:C:386:LYS:HG2	1.83	0.60
3:B:115:GLN:HE21	4:W:1:NAG:H62	1.66	0.60
1:H:36:VAL:HG21	1:H:106:ARG:HB2	1.83	0.60
2:L:114:ASN:HB2	3:A:499:PRO:HB2	1.84	0.59
1:H:64:ASN:HA	3:A:440:LYS:HD2	1.83	0.59
1:I:158:LYS:NZ	2:M:152:THR:OG1	2.34	0.59
1:J:111(A):ARG:NH2	2:N:38:TYR:OH	2.35	0.59
3:C:1129:VAL:HB	3:C:1132:ILE:HB	1.83	0.59
3:A:212:LEU:HD12	3:A:217:PRO:HB3	1.83	0.59
2:L:99:GLU:OE1	2:L:129:GLN:NE2	2.35	0.59
1:H:37:TYR:HB3	1:H:57:HIS:HE1	1.68	0.59
3:B:93:ALA:HB3	3:B:266:TYR:HB2	1.84	0.59
2:L:188:GLN:NE2	2:L:193:TYR:O	2.35	0.59
1:I:108:SER:HB2	1:I:114:THR:HB	1.84	0.59
3:C:1116:THR:HG22	3:C:1138:TYR:HB3	1.84	0.59
3:C:742:ILE:O	3:C:1000:ARG:NH2	2.36	0.59
3:C:747:THR:O	3:C:751:ASN:ND2	2.36	0.59
2:M:114:ASN:HB2	3:B:499:PRO:HB2	1.85	0.58
3:C:804:GLN:OE1	3:C:935:GLN:NE2	2.35	0.58
1:J:136:VAL:HG12	1:J:157:VAL:HG22	1.85	0.58
3:C:27:SER:HB3	3:C:64:TRP:HB3	1.84	0.58
3:B:820:ASP:OD1	3:B:824:ASN:ND2	2.36	0.58
1:H:19:LEU:HB3	1:H:91:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:109:VAL:HG13	1:I:112:VAL:HG22	1.85	0.58
3:B:642:VAL:HG12	3:B:651:ILE:HG12	1.85	0.58
3:C:1006:THR:O	3:C:1010:GLN:NE2	2.36	0.58
3:A:1116:THR:HG22	3:A:1138:TYR:HB3	1.85	0.58
3:A:742:ILE:O	3:A:1000:ARG:NH2	2.37	0.57
2:L:40:GLN:HG3	2:L:55:TYR:HA	1.86	0.57
3:A:132:GLU:OE1	3:A:164:ASN:ND2	2.37	0.57
3:C:319:ARG:NH1	3:B:737:ASP:OD2	2.38	0.57
2:L:188:GLN:HE21	2:L:194:ALA:HB2	1.69	0.57
3:C:1086:LYS:HD3	3:C:1122:VAL:HG21	1.85	0.57
3:B:83:ALA:HA	3:B:239:GLN:HG2	1.86	0.57
1:H:212:ASN:ND2	1:H:223:ASP:OD2	2.37	0.57
3:B:988:GLU:O	3:B:992:GLN:NE2	2.38	0.56
3:A:518:LEU:HD21	3:A:545:GLY:HA3	1.87	0.56
1:I:123:LEU:HB3	1:I:164:PRO:HG3	1.86	0.56
3:C:96:GLU:OE2	3:C:264:ALA:N	2.38	0.56
3:B:121:ASN:HB2	3:B:126:VAL:HG23	1.87	0.56
3:B:1116:THR:OG1	3:B:1119:ASN:ND2	2.36	0.56
3:B:111:ASP:OD1	3:B:111:ASP:N	2.39	0.56
3:A:392:PHE:N	3:A:524:VAL:O	2.35	0.56
3:C:317:ASN:HA	3:C:594:GLY:HA2	1.88	0.56
3:A:353:TRP:HZ3	3:A:355:ARG:HD3	1.71	0.56
3:A:136:CYS:HB3	3:A:139:PRO:HB3	1.88	0.56
3:A:902:MET:HE3	3:A:906:PHE:HE1	1.71	0.56
2:M:134:PRO:HB3	2:M:160:PHE:HB3	1.87	0.55
3:B:328:ARG:NH2	3:B:328:ARG:O	2.34	0.55
3:A:314:GLN:NE2	3:A:316:SER:O	2.39	0.55
2:L:168:ALA:HB3	2:L:215:GLN:HB3	1.88	0.55
1:I:34:ASN:OD1	1:I:37:TYR:OH	2.24	0.55
1:H:37:TYR:HB3	1:H:57:HIS:CE1	2.42	0.55
3:B:565:PHE:HB3	3:B:576:VAL:HG23	1.89	0.55
3:A:520:ALA:HB3	3:A:521:PRO:HD3	1.88	0.55
3:A:92:PHE:O	3:A:192:PHE:N	2.40	0.55
3:A:341:VAL:HG22	3:A:356:LYS:HD3	1.88	0.55
3:A:747:THR:O	3:A:751:ASN:ND2	2.40	0.55
3:B:329:PHE:O	3:B:580:GLN:NE2	2.40	0.55
3:B:514:SER:OG	3:B:516:GLU:OE1	2.24	0.55
1:H:115:PHE:O	2:L:52:THR:OG1	2.24	0.55
1:I:64:ASN:ND2	3:B:437:ASN:OD1	2.40	0.54
1:I:136:VAL:HG12	1:I:157:VAL:HG22	1.89	0.54
3:B:742:ILE:O	3:B:1000:ARG:NH2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:802:PHE:HD1	3:B:805:ILE:HD11	1.72	0.54
3:A:763:LEU:HD22	3:A:1008:VAL:HG21	1.89	0.54
1:H:136:VAL:HG12	1:H:157:VAL:HG22	1.89	0.54
2:N:114:ASN:ND2	3:C:499:PRO:O	2.39	0.54
3:C:501:TYR:HB3	3:C:505:HIS:HB2	1.89	0.54
3:C:763:LEU:HD22	3:C:1008:VAL:HG21	1.89	0.54
3:B:722:VAL:HG22	3:B:1065:VAL:HG22	1.89	0.54
3:C:884:SER:OG	3:C:887:THR:OG1	2.25	0.54
3:C:1047:TYR:HB2	3:C:1067:TYR:HB3	1.90	0.54
3:C:424:LYS:NZ	3:C:425:LEU:O	2.36	0.54
2:N:114:ASN:HB2	3:C:499:PRO:HB2	1.89	0.54
3:C:722:VAL:HG22	3:C:1065:VAL:HG22	1.90	0.54
3:C:726:ILE:HG12	3:C:1061:VAL:HG22	1.89	0.54
2:L:56:GLU:OE1	2:L:66:GLN:NE2	2.40	0.54
3:C:388:ASN:ND2	3:C:389:ASP:OD1	2.41	0.53
2:N:170:LYS:HA	2:N:175:PRO:HA	1.89	0.53
3:B:968:SER:OG	3:A:755:GLN:O	2.26	0.53
3:A:501:TYR:HB3	3:A:505:HIS:HB2	1.90	0.53
3:B:326:ILE:HD11	3:B:541:PHE:HB3	1.88	0.53
3:B:962:LEU:HD11	3:B:1004:LEU:HD23	1.91	0.53
1:I:40:SER:HB2	1:I:55:TYR:HB3	1.91	0.53
2:N:37:ASN:ND2	2:N:107:TYR:O	2.42	0.53
3:B:100:ILE:HD13	3:B:263:ALA:HB2	1.91	0.53
3:B:725:GLU:OE2	3:B:1028:LYS:NZ	2.39	0.53
1:I:125:THR:HG22	1:I:127:ALA:H	1.74	0.53
1:J:37:TYR:O	1:J:57:HIS:ND1	2.41	0.53
3:C:326:ILE:HD11	3:C:534:VAL:HG22	1.92	0.52
1:H:157:VAL:HB	1:H:193:LEU:HB3	1.91	0.52
2:M:79:SER:OG	2:M:88:SER:OG	2.28	0.52
3:C:206:LYS:HB2	3:C:223:LEU:HA	1.91	0.52
3:B:126:VAL:HB	3:B:174:PRO:HA	1.91	0.52
3:C:802:PHE:HD1	3:C:805:ILE:HD11	1.73	0.52
1:J:19:LEU:HB3	1:J:91:LEU:HB3	1.91	0.52
2:M:129:GLN:HB2	2:M:161:TYR:HE2	1.74	0.52
3:C:909:ILE:O	3:C:1108:ASN:ND2	2.43	0.52
3:B:518:LEU:HD11	4:Z:2:NAG:H5	1.91	0.52
3:B:1047:TYR:HB2	3:B:1067:TYR:HB3	1.92	0.52
1:J:167:VAL:HG12	1:J:213:VAL:HG12	1.91	0.51
2:N:108:ASP:OD1	2:N:109:ASN:N	2.42	0.51
3:C:1040:VAL:HG21	3:B:1035:GLY:HA3	1.93	0.51
3:C:442:ASP:O	3:C:448:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:611:LEU:HD22	3:B:666:ILE:HG23	1.92	0.51
3:A:884:SER:OG	3:A:887:THR:OG1	2.26	0.51
1:H:40:SER:HB2	1:H:55:TYR:HB3	1.92	0.51
3:C:393:THR:O	3:C:523:THR:OG1	2.28	0.51
3:A:726:ILE:HG12	3:A:1061:VAL:HG22	1.93	0.51
3:B:139:PRO:HB2	3:B:241:LEU:HD23	1.93	0.51
3:C:84:LEU:H	3:C:84:LEU:HD22	1.76	0.51
3:B:973:ILE:HG13	3:B:984:LEU:HD11	1.92	0.51
3:B:1084:ASP:OD2	3:B:1086:LYS:NZ	2.44	0.51
2:M:176:VAL:HG12	2:M:178:ALA:H	1.76	0.51
3:C:64:TRP:HE1	3:C:264:ALA:HB1	1.76	0.51
3:C:745:ASP:OD1	3:A:319:ARG:NH2	2.42	0.50
3:B:741:TYR:OH	3:B:962:LEU:O	2.26	0.50
1:I:52:TRP:CZ2	1:I:54:GLY:HA2	2.47	0.50
1:J:80:VAL:HG23	1:J:87:PHE:HB3	1.93	0.50
2:N:6:GLN:HG2	2:N:23:CYS:HB2	1.93	0.50
3:C:142:ASP:HB2	3:C:158:ARG:HE	1.76	0.50
3:B:905:ARG:NH2	3:B:1049:LEU:O	2.43	0.50
2:N:183:THR:OG1	2:N:196:SER:N	2.43	0.50
3:A:725:GLU:OE1	3:A:1064:HIS:NE2	2.44	0.50
3:A:962:LEU:HD11	3:A:1004:LEU:HD23	1.94	0.50
2:L:188:GLN:N	2:L:192:LYS:O	2.38	0.49
3:A:756:TYR:OH	3:A:994:ASP:OD1	2.27	0.49
3:C:379:CYS:HA	3:C:432:CYS:HA	1.95	0.49
3:A:354:ASN:OD1	3:A:355:ARG:N	2.44	0.49
3:C:131:CYS:HA	3:C:166:CYS:HA	1.95	0.49
3:C:770:ILE:O	3:C:774:GLN:HG2	2.13	0.49
3:A:236:THR:HG21	6:A:1301:NAG:H62	1.95	0.49
3:A:735:SER:OG	3:A:859:THR:OG1	2.28	0.49
2:M:56:GLU:OE1	2:M:66:GLN:NE2	2.46	0.49
3:A:948:LEU:HD21	3:A:1059:GLY:HA3	1.94	0.49
3:C:112:SER:OG	3:C:132:GLU:OE1	2.30	0.49
3:C:825:LYS:NZ	3:C:938:LEU:O	2.36	0.49
2:M:95:LYS:HG3	2:M:97:GLU:HG2	1.95	0.49
2:M:188:GLN:N	2:M:192:LYS:O	2.43	0.49
3:A:97:LYS:H	3:A:97:LYS:HD2	1.77	0.49
3:C:889:GLY:O	3:A:1045:LYS:NZ	2.38	0.49
1:I:25:VAL:HG21	1:I:30:ILE:HD11	1.95	0.49
3:A:119:ILE:HG12	3:A:128:ILE:HG23	1.94	0.49
2:L:95:LYS:HG3	2:L:97:GLU:HG2	1.95	0.48
1:I:19:LEU:HB2	1:I:94:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:39:VAL:N	2:N:57:ASN:OD1	2.45	0.48
3:C:88:ASP:N	3:C:88:ASP:OD1	2.46	0.48
2:L:57:ASN:HD22	2:L:80:ILE:HG13	1.78	0.48
1:I:115:PHE:O	2:M:52:THR:OG1	2.31	0.48
3:C:985:ASP:OD1	3:C:985:ASP:N	2.43	0.48
3:A:770:ILE:O	3:A:774:GLN:HG2	2.13	0.48
3:B:676:THR:HA	3:B:690:GLN:HA	1.95	0.48
1:H:166:THR:OG1	1:H:214:ASN:N	2.47	0.48
3:B:770:ILE:O	3:B:774:GLN:HG2	2.13	0.48
3:C:102:ARG:O	3:C:121:ASN:N	2.39	0.48
3:C:642:VAL:HG12	3:C:651:ILE:HG12	1.95	0.48
3:A:455:LEU:HD23	3:A:489:TYR:HB3	1.96	0.48
1:J:37:TYR:HB3	1:J:57:HIS:CE1	2.48	0.48
3:B:95:THR:HB	3:B:189:LEU:HD13	1.96	0.48
3:B:645:THR:OG1	3:B:648:GLY:O	2.32	0.48
3:A:30:ASN:OD1	3:A:31:SER:N	2.46	0.48
1:J:40:SER:HB2	1:J:55:TYR:HB3	1.95	0.48
3:B:661:GLU:O	3:B:695:TYR:OH	2.26	0.48
3:A:567:ARG:NH2	3:A:571:ASP:O	2.45	0.48
3:C:895:GLN:NE2	3:A:706:ALA:O	2.47	0.48
3:B:820:ASP:O	3:B:824:ASN:ND2	2.33	0.48
1:H:171:SER:HB2	3:B:417:ASN:HD22	1.78	0.47
3:B:319:ARG:NH2	3:A:745:ASP:OD1	2.46	0.47
3:B:735:SER:HA	3:B:767:LEU:HD13	1.95	0.47
2:N:13:GLU:HG2	2:N:19:VAL:HG22	1.96	0.47
3:C:1005:GLN:OE1	3:A:1002:GLN:NE2	2.41	0.47
2:N:134:PRO:HB3	2:N:160:PHE:HB3	1.96	0.47
3:C:895:GLN:HE22	3:A:706:ALA:HB3	1.80	0.47
3:A:424:LYS:NZ	3:A:425:LEU:O	2.40	0.47
3:C:747:THR:HG22	3:C:751:ASN:HD21	1.79	0.47
1:I:3:GLN:O	1:I:26:SER:OG	2.31	0.47
3:B:659:SER:HB3	3:B:698:SER:HB3	1.96	0.47
3:B:666:ILE:HD11	3:B:672:ALA:HB2	1.96	0.47
1:J:116:ASP:OD1	1:J:116:ASP:N	2.41	0.47
1:J:184:VAL:HB	2:N:183:THR:HG22	1.95	0.47
3:C:350:VAL:HG22	3:C:422:ASN:HB3	1.97	0.47
3:A:66:HIS:HA	3:A:264:ALA:HA	1.95	0.47
3:A:358:ILE:HB	3:A:395:VAL:HB	1.97	0.47
3:A:676:THR:HG22	3:A:690:GLN:HG2	1.96	0.47
1:J:71:LEU:HD22	1:J:75:ARG:HH11	1.80	0.47
2:N:19:VAL:HB	2:N:91:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:VAL:HG13	1:H:112:VAL:HG22	1.97	0.47
3:B:310:LYS:HG3	3:B:600:PRO:HA	1.97	0.47
3:A:214:ARG:O	3:A:266:TYR:OH	2.31	0.47
1:H:116:ASP:OD1	1:H:116:ASP:N	2.43	0.46
1:J:108:SER:HB2	1:J:114:THR:HB	1.97	0.46
3:B:424:LYS:NZ	3:B:425:LEU:O	2.39	0.46
3:B:756:TYR:OH	3:B:994:ASP:OD1	2.28	0.46
3:A:379:CYS:HA	3:A:432:CYS:HA	1.97	0.46
3:C:287:ASP:OD1	3:C:288:ALA:N	2.48	0.46
3:C:930:ALA:O	3:C:934:ILE:HG12	2.15	0.46
3:B:418:ILE:HA	3:B:422:ASN:HD22	1.80	0.46
3:A:37:TYR:OH	3:A:54:LEU:O	2.29	0.46
3:A:393:THR:HG23	3:A:521:PRO:HG2	1.97	0.46
1:I:109:VAL:HG12	3:B:502:GLY:HA2	1.97	0.46
1:J:52:TRP:CZ2	1:J:54:GLY:HA2	2.50	0.46
3:A:30:ASN:ND2	3:A:215:ASP:O	2.47	0.46
3:A:109:THR:HA	3:A:237:ARG:HE	1.80	0.46
3:A:117:LEU:HD12	3:A:119:ILE:HG13	1.97	0.46
1:H:134:PRO:HB3	1:H:160:TYR:HB3	1.98	0.46
3:C:83:ALA:HA	3:C:239:GLN:HE21	1.80	0.46
3:A:353:TRP:HB3	3:A:400:PHE:HB3	1.97	0.46
1:I:111(A):ARG:CZ	1:I:111(A):ARG:H	2.29	0.46
1:I:116:ASP:OD1	1:I:116:ASP:N	2.42	0.46
3:B:880:GLY:O	3:B:884:SER:OG	2.30	0.46
3:B:985:ASP:OD1	3:B:985:ASP:N	2.44	0.46
3:A:329:PHE:O	3:A:580:GLN:NE2	2.33	0.46
3:A:802:PHE:HD1	3:A:805:ILE:HD11	1.80	0.46
1:I:106:ARG:HD3	1:I:117:TYR:HB2	1.97	0.46
3:A:882:ILE:HG13	3:A:883:THR:HG23	1.97	0.46
3:A:969:LYS:HB3	3:A:975:SER:HB3	1.97	0.46
1:H:21:LEU:HD11	1:H:124:VAL:HG21	1.98	0.46
3:C:193:VAL:HG23	3:C:223:LEU:HD22	1.97	0.46
3:C:386:LYS:HE2	3:C:390:LEU:HD11	1.97	0.46
3:A:350:VAL:HG22	3:A:422:ASN:HB3	1.96	0.46
1:I:184:VAL:HB	2:M:183:THR:HG22	1.97	0.45
3:C:773:GLU:OE2	3:C:1019:ARG:NE	2.45	0.45
3:A:201:PHE:HB3	3:A:229:LEU:HB2	1.97	0.45
3:A:642:VAL:HG12	3:A:651:ILE:HG12	1.98	0.45
3:A:1094:VAL:N	3:A:1105:THR:O	2.46	0.45
1:I:151:ALA:HB3	1:I:204:LEU:HD21	1.98	0.45
3:B:699:LEU:HD21	3:A:869:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:83:ALA:HB1	3:A:237:ARG:HD3	1.99	0.45
3:A:109:THR:OG1	3:A:111:ASP:OD1	2.30	0.45
3:C:294:ASP:OD1	3:C:294:ASP:N	2.47	0.45
3:C:725:GLU:OE1	3:C:1064:HIS:NE2	2.49	0.45
1:I:80:VAL:HG23	1:I:87:PHE:HB3	1.98	0.45
2:N:171:ALA:HB2	2:N:176:VAL:HG22	1.99	0.45
3:C:342:PHE:HE1	3:C:434:ILE:HG21	1.82	0.45
3:C:211:ASN:C	3:C:213:GLU:H	2.24	0.45
3:B:40:ASP:OD1	3:B:40:ASP:N	2.47	0.45
3:C:895:GLN:HG2	3:A:713:ALA:HB2	1.99	0.45
3:A:396:TYR:HB2	3:A:514:SER:HB3	1.98	0.45
1:H:52:TRP:CZ2	1:H:54:GLY:HA2	2.51	0.45
3:B:204:TYR:HB3	3:B:223:LEU:HB3	1.98	0.45
3:B:712:ILE:HD13	3:B:1094:VAL:HG11	1.99	0.45
1:J:18:THR:HA	1:J:92:ASN:HA	2.00	0.44
1:J:31:ARG:NH2	1:J:82:THR:O	2.50	0.44
1:J:38:TYR:CD1	1:J:109:VAL:HG21	2.51	0.44
3:C:53:ASP:OD1	3:C:54:LEU:N	2.44	0.44
3:C:106:PHE:HB2	3:C:117:LEU:HD23	1.99	0.44
3:C:355:ARG:HB2	3:C:466:ARG:HH12	1.81	0.44
3:B:19:ILE:HG22	3:B:81:ASN:H	1.82	0.44
1:I:56:ILE:HG13	1:I:65:THR:HG22	1.99	0.44
3:C:127:VAL:HG11	3:C:129:LYS:HE3	2.00	0.44
3:B:1081:ILE:HG23	3:B:1135:ASN:HB3	2.00	0.44
1:I:37:TYR:HD2	1:I:57:HIS:HE1	1.64	0.44
1:I:141:PRO:HB3	1:I:153:LEU:HB3	1.99	0.44
1:J:42:ILE:O	1:J:103:TYR:N	2.44	0.44
3:C:106:PHE:HB2	3:C:117:LEU:HB3	2.00	0.44
3:C:139:PRO:HB2	3:C:159:VAL:HG12	1.99	0.44
4:K:1:NAG:H61	4:K:2:NAG:N2	2.32	0.44
3:C:937:SER:O	3:C:941:THR:OG1	2.23	0.44
3:B:1074:ASN:HB3	3:A:895:GLN:HE21	1.83	0.44
1:J:161:PHE:HB3	1:J:162:PRO:HD3	2.00	0.44
3:A:231:ILE:HG12	3:A:233:ILE:HG23	1.98	0.44
2:L:134:PRO:HB3	2:L:160:PHE:HB3	1.99	0.44
2:M:39:VAL:N	2:M:57:ASN:OD1	2.46	0.44
2:N:137:THR:HB	2:N:156:LEU:HB2	2.00	0.44
3:C:31:SER:HB3	3:C:62:VAL:HG21	2.00	0.44
3:C:1011:GLN:OE1	3:C:1014:ARG:NH1	2.50	0.44
3:B:980:ILE:HD13	3:B:992:GLN:HB3	2.00	0.44
3:B:988:GLU:HG3	3:B:992:GLN:HE22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:20:THR:HA	2:M:90:THR:HA	2.00	0.43
3:C:328:ARG:NH1	3:C:531:THR:O	2.50	0.43
3:A:722:VAL:HG22	3:A:1065:VAL:HG22	1.99	0.43
2:L:108:ASP:HB3	2:L:115:VAL:HB	2.00	0.43
1:J:59:SER:OG	1:J:64:ASN:ND2	2.51	0.43
3:C:170:TYR:CE2	3:C:172:SER:HB2	2.53	0.43
1:H:110:GLY:HA2	3:A:503:VAL:HG12	2.00	0.43
1:I:19:LEU:HB3	1:I:91:LEU:HB3	2.00	0.43
3:A:717:ASN:HD22	3:A:1071:GLN:CD	2.26	0.43
1:I:111(A):ARG:O	3:B:502:GLY:N	2.48	0.43
3:B:115:GLN:HA	3:B:132:GLU:HB3	2.01	0.43
2:N:126:VAL:HB	2:N:129:GLN:HE21	1.82	0.43
3:B:19:ILE:HG12	3:B:20:THR:H	1.83	0.43
3:B:988:GLU:HG3	3:B:992:GLN:NE2	2.33	0.43
3:B:1097:SER:HB2	3:B:1102:TRP:CD2	2.53	0.43
1:J:170:ASN:ND2	1:J:207:GLN:OE1	2.49	0.43
3:A:455:LEU:HG	3:A:456:LEU:HD12	1.99	0.43
2:N:159:ASP:HA	2:N:192:LYS:HD2	2.00	0.43
3:C:962:LEU:HD11	3:C:1004:LEU:HD23	2.01	0.43
3:B:66:HIS:HA	3:B:264:ALA:HA	2.00	0.43
1:H:71:LEU:HD22	1:H:75:ARG:HH11	1.83	0.43
1:J:56:ILE:HG13	1:J:65:THR:HG22	2.01	0.43
3:C:117:LEU:HD13	3:C:130:VAL:HG22	2.01	0.43
3:C:882:ILE:HG13	3:C:883:THR:HG23	2.00	0.43
1:H:138:PRO:HA	1:H:155:CYS:HA	2.00	0.43
3:B:1040:VAL:HG21	3:A:1035:GLY:HA3	2.01	0.43
3:A:422:ASN:HD21	3:A:454:ARG:N	2.14	0.43
1:I:215:HIS:O	1:I:219:ASN:N	2.50	0.43
3:C:142:ASP:OD2	3:C:158:ARG:NH1	2.45	0.43
3:C:981:LEU:O	3:A:386:LYS:NZ	2.51	0.43
3:B:96:GLU:HG2	3:B:98:SER:H	1.83	0.43
3:B:197:ILE:HG22	3:B:200:TYR:O	2.19	0.43
2:N:168:ALA:HB3	2:N:215:GLN:HB3	2.00	0.42
3:C:86:PHE:CZ	3:C:89:GLY:HA2	2.54	0.42
3:B:121:ASN:HD21	3:B:174:PRO:HB3	1.84	0.42
3:B:599:THR:HB	3:B:608:VAL:HG12	1.99	0.42
3:B:1045:LYS:NZ	3:A:889:GLY:O	2.42	0.42
3:C:299:THR:HA	3:C:302:THR:HG22	2.01	0.42
3:B:770:ILE:HD11	3:B:1012:LEU:HD23	2.01	0.42
3:B:1089:PHE:HZ	3:B:1129:VAL:HG21	1.84	0.42
3:A:89:GLY:HA3	3:A:270:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:808:ASP:OD1	3:A:810:SER:OG	2.37	0.42
3:C:1035:GLY:HA3	3:A:1040:VAL:HG21	2.01	0.42
3:A:110:LEU:HG	3:A:237:ARG:HD2	2.01	0.42
2:M:105:GLN:HE21	2:M:116:ALA:HB1	1.84	0.42
1:J:35:GLU:HG3	1:J:36:VAL:HG13	2.01	0.42
3:C:917:TYR:HB3	3:A:1129:VAL:HG13	2.01	0.42
3:B:334:ASN:O	3:B:334:ASN:ND2	2.52	0.42
3:A:327:VAL:HG21	3:A:528:LYS:HE3	2.02	0.42
3:C:557:LYS:HD2	3:C:559:PHE:HE1	1.84	0.42
3:B:736:VAL:HA	3:B:858:LEU:HA	2.00	0.42
3:A:905:ARG:NH2	3:A:1049:LEU:O	2.47	0.42
3:C:231:ILE:HG22	3:C:233:ILE:HG23	2.01	0.42
3:C:756:TYR:OH	3:C:994:ASP:OD1	2.33	0.42
3:C:30:ASN:OD1	3:C:31:SER:N	2.53	0.42
3:C:452:LEU:HA	3:C:494:SER:HA	2.01	0.42
3:C:964:LYS:NZ	3:A:571:ASP:OD2	2.50	0.42
3:A:718:PHE:HE1	3:A:923:ILE:HG12	1.84	0.42
1:I:168:SER:HB3	1:I:212:ASN:HB2	2.02	0.42
3:C:91:TYR:N	3:C:268:GLY:O	2.44	0.42
3:B:129:LYS:HE2	3:B:169:GLU:HG3	2.02	0.42
3:B:808:ASP:OD1	3:B:808:ASP:N	2.52	0.42
3:C:109:THR:HG22	3:C:110:LEU:HD23	2.02	0.42
3:B:128:ILE:HB	3:B:170:TYR:HB3	2.02	0.42
3:A:118:LEU:HD23	3:A:129:LYS:HD3	2.02	0.42
1:I:150:THR:HA	1:I:200:PRO:HA	2.00	0.42
3:A:132:GLU:HB3	3:A:164:ASN:HD22	1.85	0.42
2:N:99:GLU:HB2	2:N:126:VAL:HG23	2.02	0.41
3:B:197:ILE:HD12	3:B:197:ILE:HA	1.91	0.41
3:B:294:ASP:N	3:B:294:ASP:OD1	2.53	0.41
1:J:14:SER:HB3	1:J:17:GLN:HG3	2.01	0.41
3:C:566:GLY:HA2	3:B:43:PHE:H	1.86	0.41
3:B:85:PRO:HA	3:B:237:ARG:HD3	2.03	0.41
2:M:99:GLU:HA	2:M:124:LEU:HD22	2.03	0.41
3:C:19:ILE:HD12	3:C:242:LEU:HD12	2.02	0.41
3:C:770:ILE:HD11	3:C:1012:LEU:HD23	2.01	0.41
3:A:954:HIS:HA	3:A:957:GLN:HG2	2.03	0.41
2:N:53:VAL:HG12	2:N:54:ILE:HG12	2.01	0.41
3:C:1142:GLN:HG3	3:C:1143:PRO:HD3	2.03	0.41
3:A:1097:SER:HB2	3:A:1102:TRP:CD2	2.56	0.41
2:L:137:THR:O	2:L:156:LEU:N	2.51	0.41
1:I:65:THR:H	3:B:440:LYS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:105:ILE:HD13	3:B:135:PHE:CE1	2.56	0.41
3:B:358:ILE:HB	3:B:395:VAL:HB	2.03	0.41
3:B:457:ARG:NH1	3:B:459:SER:OG	2.54	0.41
3:B:986:PRO:N	3:B:987:PRO:HD2	2.35	0.41
1:I:163:GLU:HB3	1:I:164:PRO:HD3	2.03	0.41
2:M:96:THR:HA	2:M:126:VAL:HG21	2.03	0.41
2:M:168:ALA:HB3	2:M:215:GLN:HB3	2.03	0.41
3:C:173:GLN:HG2	3:C:174:PRO:HD2	2.03	0.41
3:B:720:ILE:HG13	3:B:923:ILE:HG12	2.02	0.41
3:C:35:GLY:HA3	3:C:56:LEU:HB3	2.03	0.41
3:C:104:TRP:HB3	3:C:238:PHE:HE1	1.86	0.41
3:C:611:LEU:HD22	3:C:666:ILE:HG23	2.02	0.41
3:C:934:ILE:HD13	3:C:934:ILE:HA	1.93	0.41
3:B:350:VAL:HG22	3:B:422:ASN:HB3	2.03	0.41
3:B:616:ASN:OD1	3:B:617:CYS:N	2.54	0.41
2:L:183:THR:OG1	2:L:196:SER:N	2.51	0.41
1:I:161:PHE:HB3	1:I:162:PRO:HD3	2.03	0.41
3:C:862:PRO:HA	3:C:863:PRO:HD3	1.97	0.41
3:A:903:ALA:HB1	3:A:913:GLN:HG2	2.02	0.41
3:C:1142:GLN:N	3:C:1143:PRO:HD2	2.36	0.40
3:B:319:ARG:NH1	3:A:740:MET:HB2	2.37	0.40
3:A:102:ARG:HA	3:A:121:ASN:HB2	2.03	0.40
3:A:233:ILE:H	3:A:233:ILE:HD13	1.86	0.40
1:J:163:GLU:O	1:J:165:VAL:N	2.54	0.40
1:J:77:ALA:HB3	1:J:90:LYS:HB2	2.04	0.40
3:C:736:VAL:HA	3:C:858:LEU:HA	2.04	0.40
3:B:127:VAL:HA	3:B:171:VAL:HG12	2.03	0.40
3:B:906:PHE:HA	3:B:909:ILE:HG12	2.04	0.40
3:A:307:THR:HA	3:A:602:THR:HG21	2.03	0.40
3:A:1028:LYS:HB2	3:A:1028:LYS:HE2	1.86	0.40
2:N:176:VAL:HG12	2:N:178:ALA:H	1.87	0.40
3:C:552:LEU:HD12	3:C:585:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	210/453 (46%)	196 (93%)	14 (7%)	0	100	100
1	I	210/453 (46%)	198 (94%)	12 (6%)	0	100	100
1	J	210/453 (46%)	199 (95%)	11 (5%)	0	100	100
2	L	213/217 (98%)	206 (97%)	7 (3%)	0	100	100
2	M	213/217 (98%)	204 (96%)	9 (4%)	0	100	100
2	N	213/217 (98%)	203 (95%)	10 (5%)	0	100	100
3	A	1004/1295 (78%)	957 (95%)	47 (5%)	0	100	100
3	B	1006/1295 (78%)	956 (95%)	50 (5%)	0	100	100
3	C	1003/1295 (78%)	968 (96%)	35 (4%)	0	100	100
All	All	4282/5895 (73%)	4087 (95%)	195 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	182/404 (45%)	180 (99%)	2 (1%)	70	83
1	I	182/404 (45%)	177 (97%)	5 (3%)	40	64
1	J	182/404 (45%)	181 (100%)	1 (0%)	86	93
2	L	186/188 (99%)	186 (100%)	0	100	100
2	M	186/188 (99%)	185 (100%)	1 (0%)	86	93
2	N	186/188 (99%)	185 (100%)	1 (0%)	86	93
3	A	895/1118 (80%)	874 (98%)	21 (2%)	45	69
3	B	897/1118 (80%)	864 (96%)	33 (4%)	29	54
3	C	896/1118 (80%)	870 (97%)	26 (3%)	37	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3792/5130 (74%)	3702 (98%)	90 (2%)	45 68

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	126	VAL
1	H	160	TYR
1	I	38	TYR
1	I	107	VAL
1	I	109	VAL
1	I	111(A)	ARG
1	I	209	TYR
2	M	23	CYS
1	J	107	VAL
2	N	23	CYS
3	C	18	LEU
3	C	61	ASN
3	C	95	THR
3	C	108	THR
3	C	113	LYS
3	C	126	VAL
3	C	136	CYS
3	C	143	VAL
3	C	210	ILE
3	C	212	LEU
3	C	214	ARG
3	C	231	ILE
3	C	233	ILE
3	C	312	ILE
3	C	456	LEU
3	C	468	ILE
3	C	478	LYS
3	C	564	GLN
3	C	585	LEU
3	C	650	LEU
3	C	753	LEU
3	C	858	LEU
3	C	966	LEU
3	C	1010	GLN
3	C	1045	LYS
3	C	1104	VAL
3	B	19	ILE

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Mol	Chain	Res	Type
3	B	110	LEU
3	B	111	ASP
3	B	131	CYS
3	B	135	PHE
3	B	165	ASN
3	B	214	ARG
3	B	229	LEU
3	B	244	LEU
3	B	312	ILE
3	B	320	VAL
3	B	328	ARG
3	B	332	ILE
3	B	456	LEU
3	B	468	ILE
3	B	524	VAL
3	B	529	LYS
3	B	535	LYS
3	B	538	CYS
3	B	569	ILE
3	B	590	CYS
3	B	615	VAL
3	B	650	LEU
3	B	753	LEU
3	B	825	LYS
3	B	856	ASN
3	B	858	LEU
3	B	923	ILE
3	B	992	GLN
3	B	1100	THR
3	B	1104	VAL
3	B	1122	VAL
3	B	1130	ILE
3	A	97	LYS
3	A	105	ILE
3	A	117	LEU
3	A	120	VAL
3	A	131	CYS
3	A	231	ILE
3	A	233	ILE
3	A	312	ILE
3	A	332	ILE
3	A	468	ILE

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Mol	Chain	Res	Type
3	A	478	LYS
3	A	525	CYS
3	A	546	LEU
3	A	595	VAL
3	A	716	THR
3	A	738	CYS
3	A	753	LEU
3	A	854	LYS
3	A	931	ILE
3	A	1083	HIS
3	A	1125	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
2	L	191	ASN
2	L	218	HIS
1	I	3	GLN
2	M	40	GLN
2	M	66	GLN
2	M	105	GLN
2	M	188	GLN
2	M	215	GLN
1	J	3	GLN
1	J	92	ASN
2	N	37	ASN
2	N	40	GLN
2	N	43	GLN
2	N	105	GLN
2	N	188	GLN
2	N	209	HIS
2	N	218	HIS
3	C	23	GLN
3	C	52	HIS
3	C	188	ASN
3	C	196	ASN
3	C	211	ASN
3	C	360	ASN
3	C	540	ASN
3	C	751	ASN
3	C	755	GLN

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Mol	Chain	Res	Type
3	C	913	GLN
3	C	919	ASN
3	C	1071	GLN
3	C	1083	HIS
3	C	1088	HIS
3	C	1135	ASN
3	B	211	ASN
3	B	334	ASN
3	B	417	ASN
3	B	675	GLN
3	B	703	ASN
3	B	755	GLN
3	B	919	ASN
3	B	957	GLN
3	B	992	GLN
3	B	1002	GLN
3	B	1048	HIS
3	A	49	HIS
3	A	115	GLN
3	A	164	ASN
3	A	218	GLN
3	A	321	GLN
3	A	564	GLN
3	A	603	ASN
3	A	607	GLN
3	A	613	GLN
3	A	675	GLN
3	A	690	GLN
3	A	762	GLN
3	A	787	GLN
3	A	926	GLN
3	A	935	GLN
3	A	955	ASN
3	A	960	ASN
3	A	1010	GLN
3	A	1135	ASN
3	A	1142	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

43 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	1	4,3	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	D	2	4	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	E	1	4,3	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	E	2	4	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	F	1	3,5	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	F	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	BMA	F	3	5	11,11,12	0.59	0	15,15,17	0.76	0
4	NAG	G	1	4,3	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	K	1	4,3	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	K	2	4	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	O	1	4,3	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	O	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	P	1	4,3	14,14,15	0.28	0	17,19,21	0.55	0
4	NAG	P	2	4	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	Q	1	4,3	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	Q	2	4	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	R	1	4,3	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	R	2	4	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	S	1	4,3	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	S	2	4	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	T	1	4,3	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	T	2	4	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	U	1	4,3	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	U	2	4	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	V	1	4,3	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	V	2	4	14,14,15	0.25	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	W	1	4,3	14,14,15	0.31	0	17,19,21	0.54	0
4	NAG	W	2	4	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	X	1	4,3	14,14,15	0.31	0	17,19,21	0.58	0
4	NAG	X	2	4	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	Y	1	4,3	14,14,15	0.32	0	17,19,21	0.58	0
4	NAG	Y	2	4	14,14,15	0.27	0	17,19,21	0.43	0
4	NAG	Z	1	4,3	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	Z	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	a	1	4,3	14,14,15	0.22	0	17,19,21	0.36	0
4	NAG	a	2	4	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	b	1	4,3	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	b	2	4	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	c	1	4,3	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	c	2	4	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	d	1	4,3	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	d	2	4	14,14,15	0.23	0	17,19,21	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	R	1	4,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	1/6/23/26	0/1/1/1
4	NAG	V	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1
4	NAG	X	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	1	4,3	-	3/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	NAG	a	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	0/6/23/26	0/1/1/1
4	NAG	b	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1
4	NAG	c	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1
4	NAG	d	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6

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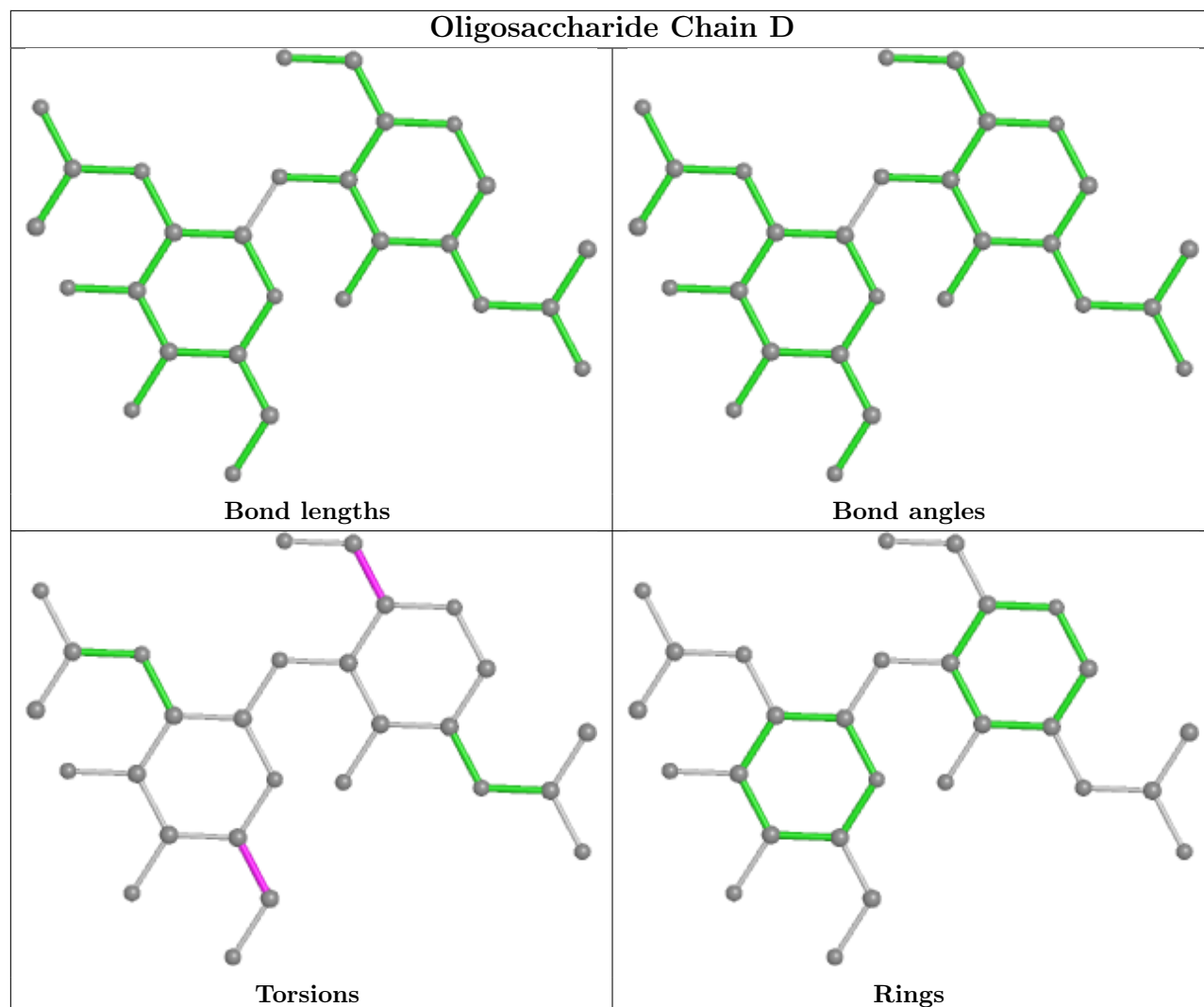
Mol	Chain	Res	Type	Atoms
4	b	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	P	1	NAG	C3-C2-N2-C7
4	T	1	NAG	C3-C2-N2-C7
4	U	2	NAG	C3-C2-N2-C7
4	X	1	NAG	C3-C2-N2-C7
4	Y	1	NAG	C3-C2-N2-C7
4	U	1	NAG	O5-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6

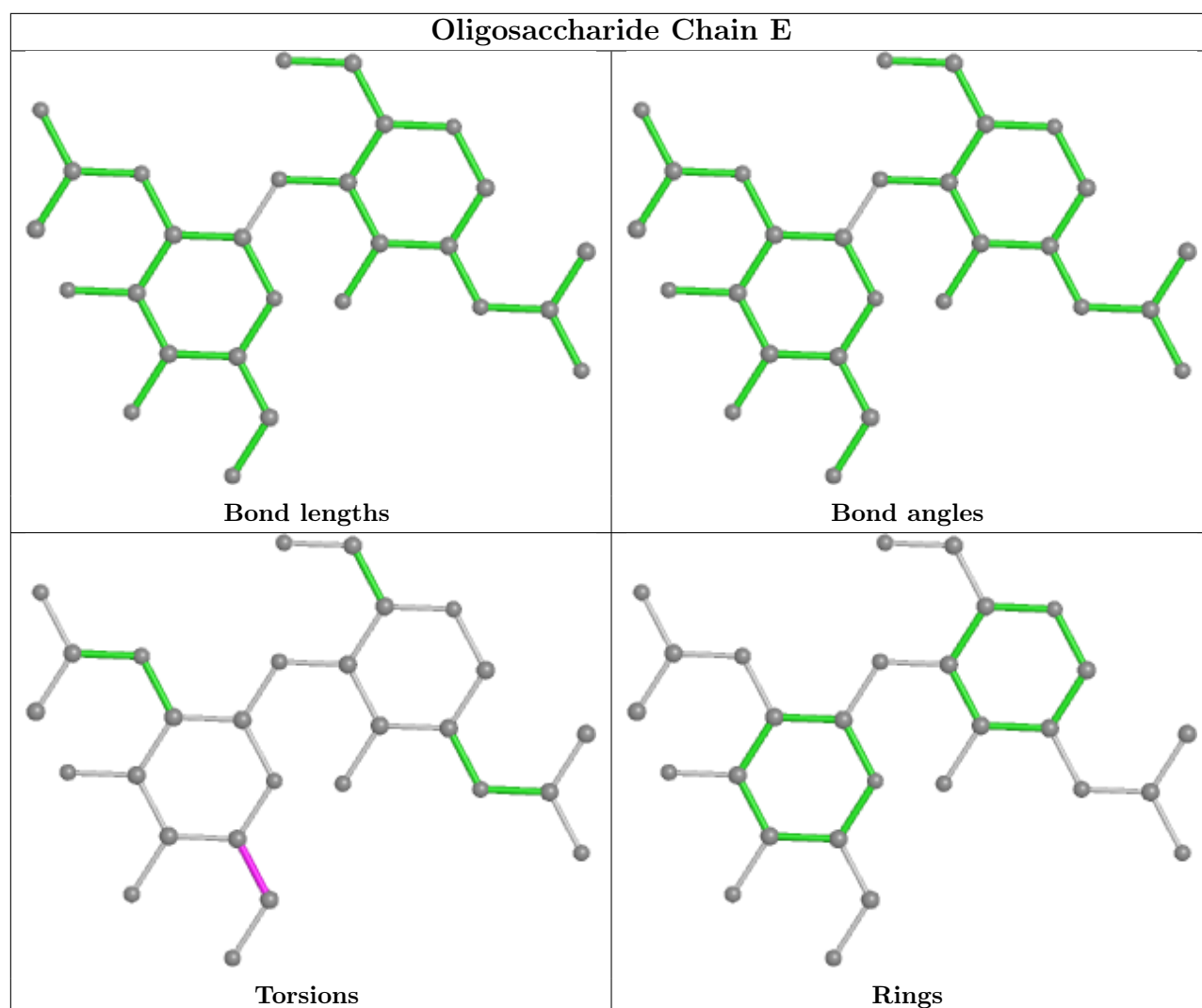
There are no ring outliers.

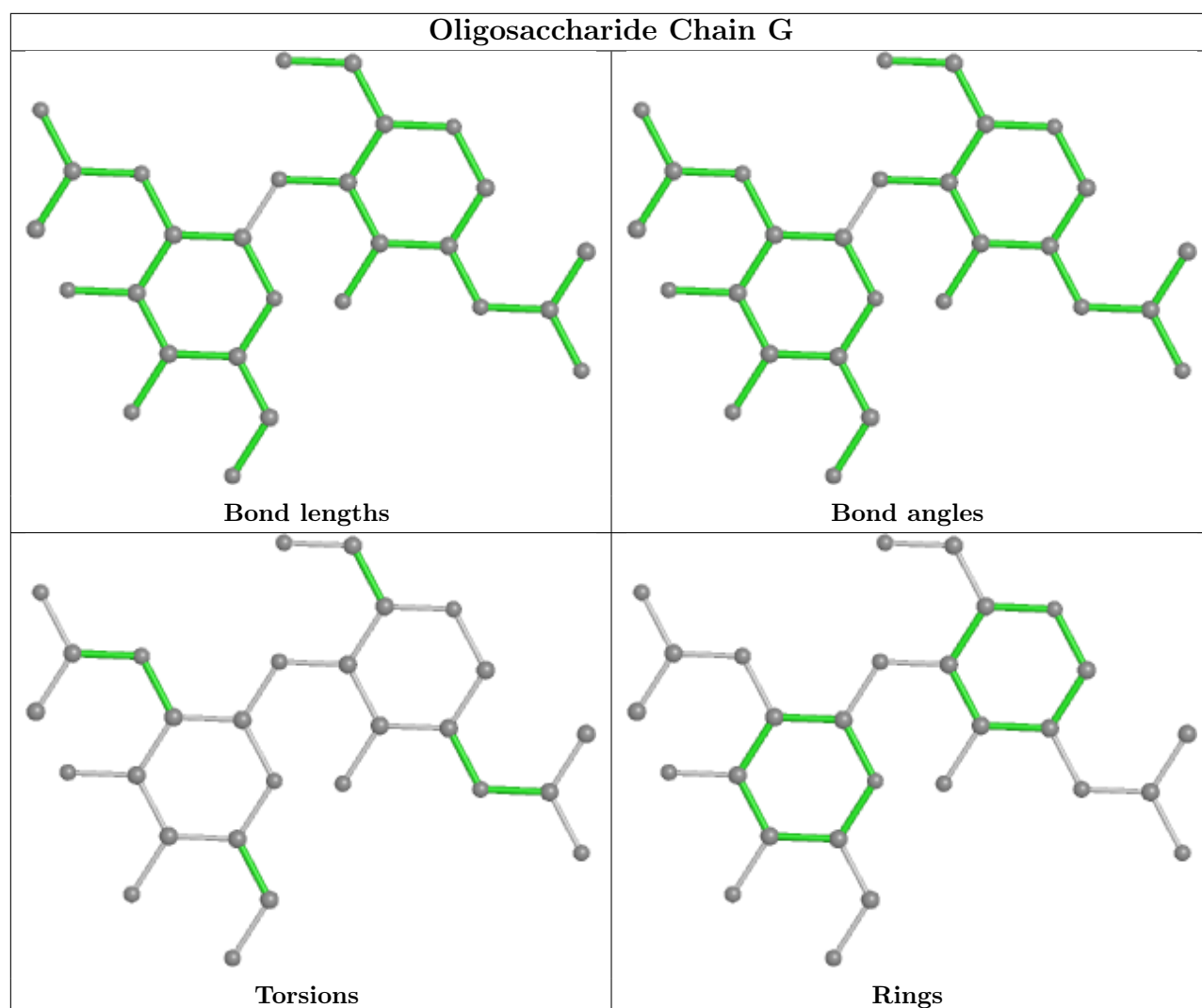
4 monomers are involved in 3 short contacts:

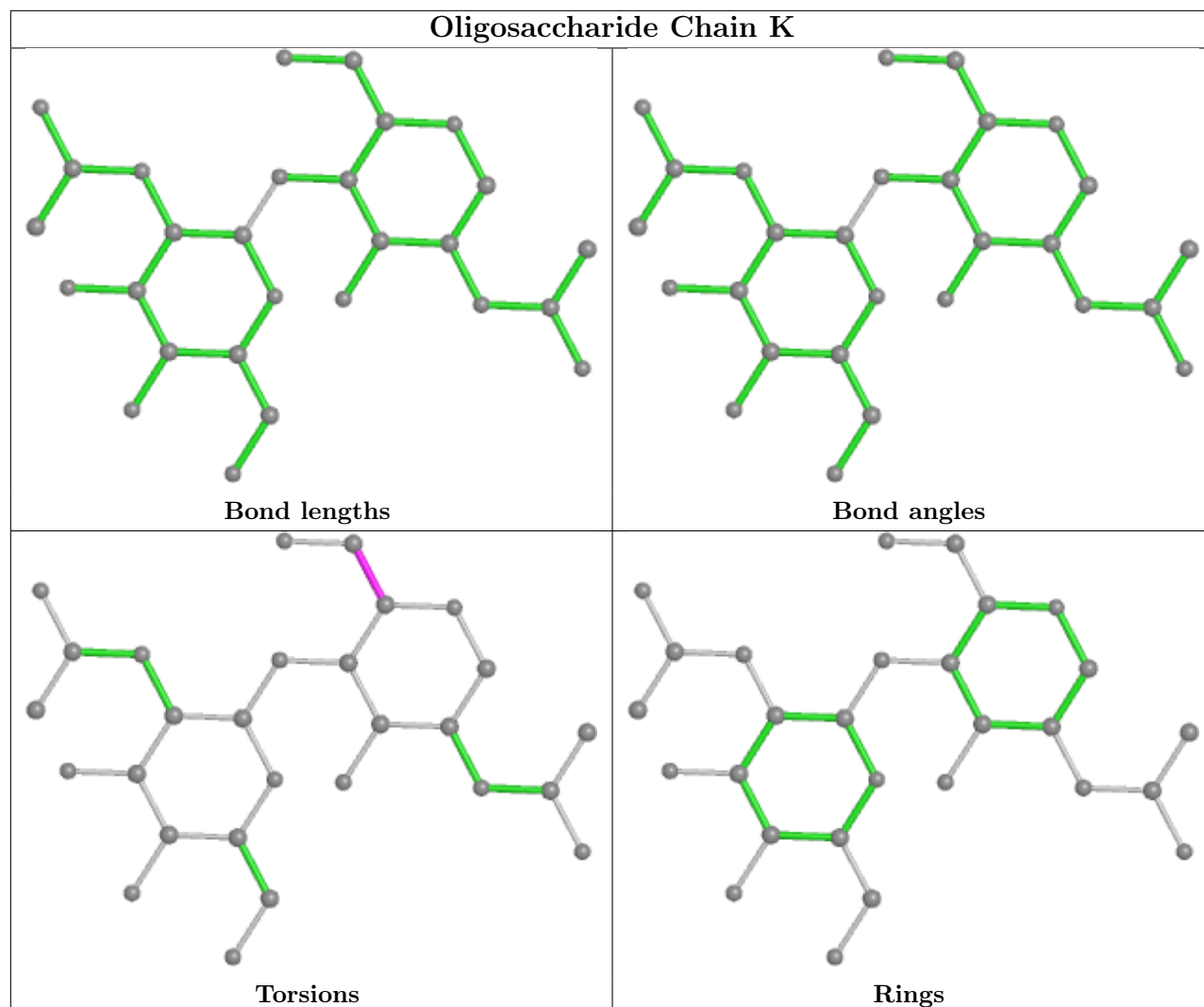
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	2	NAG	1	0
4	W	1	NAG	1	0
4	K	1	NAG	1	0
4	Z	2	NAG	1	0

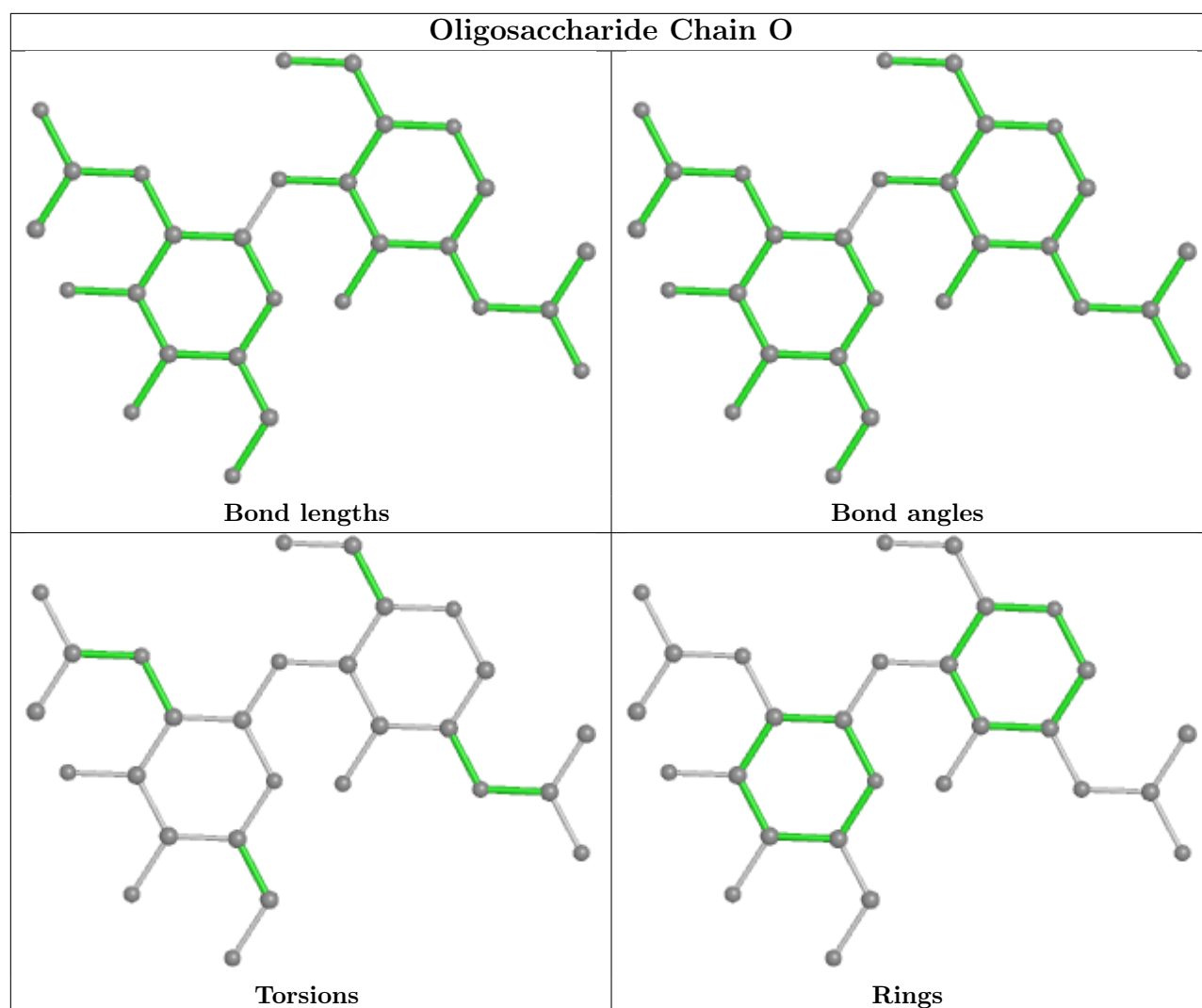
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

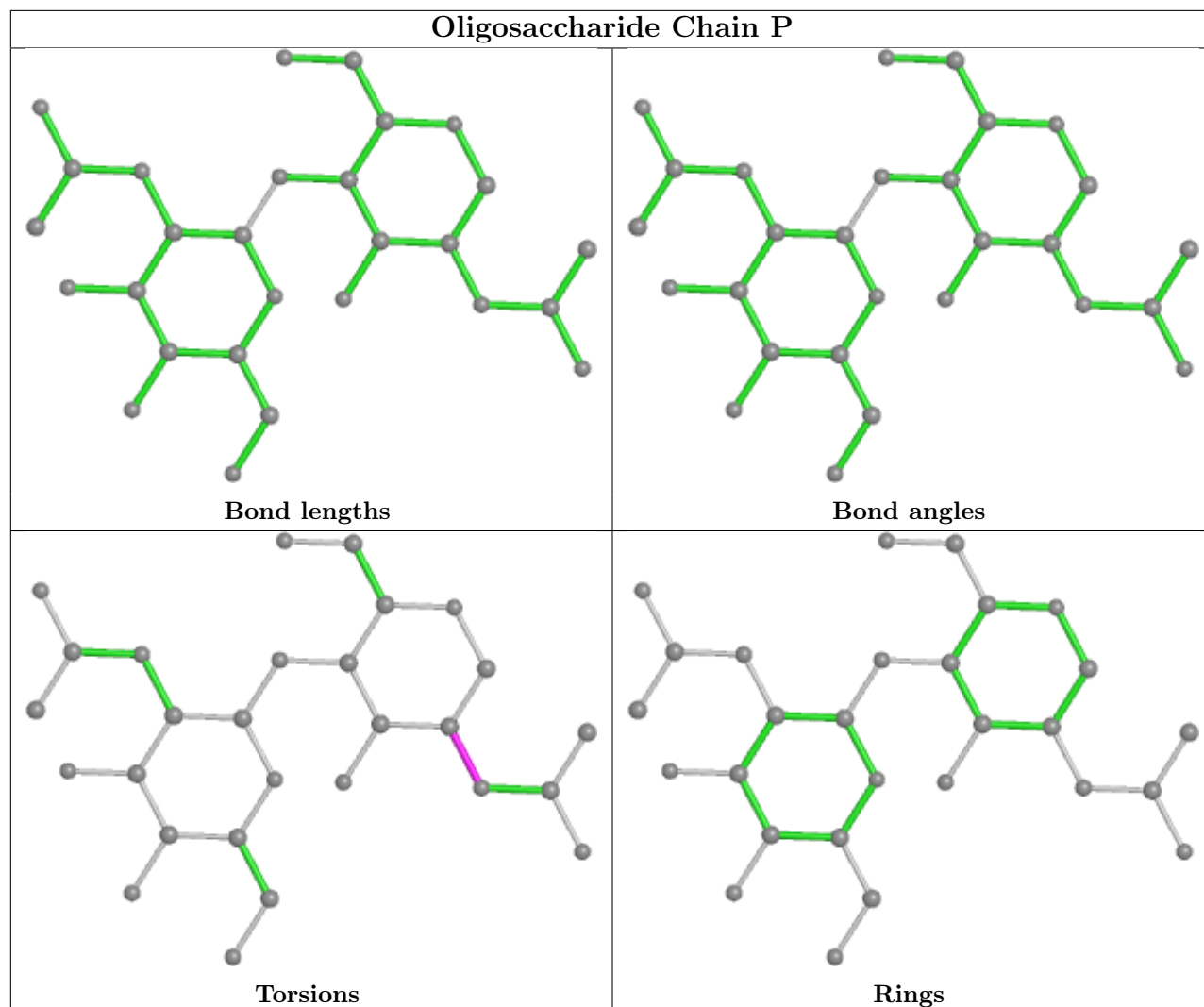


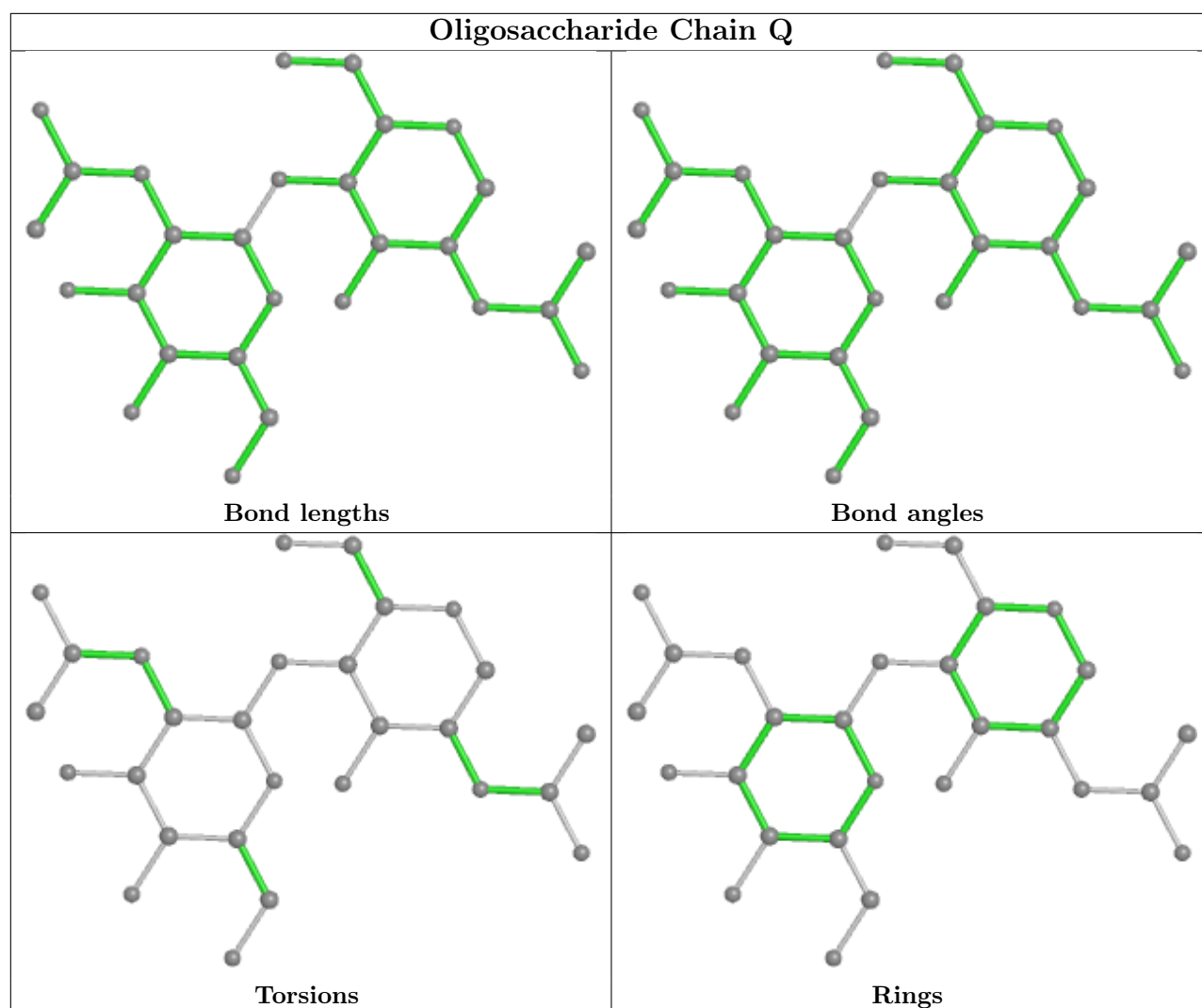


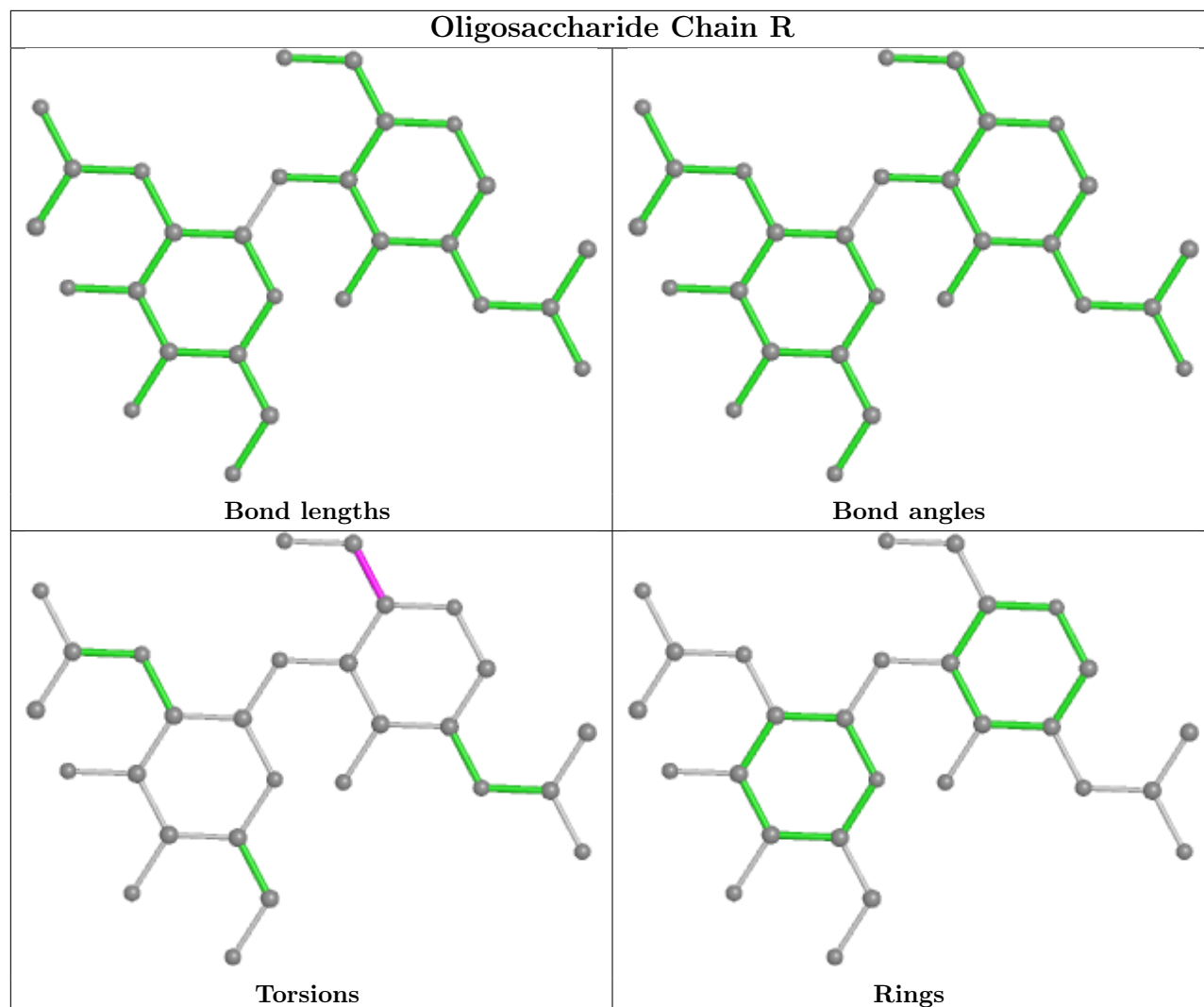


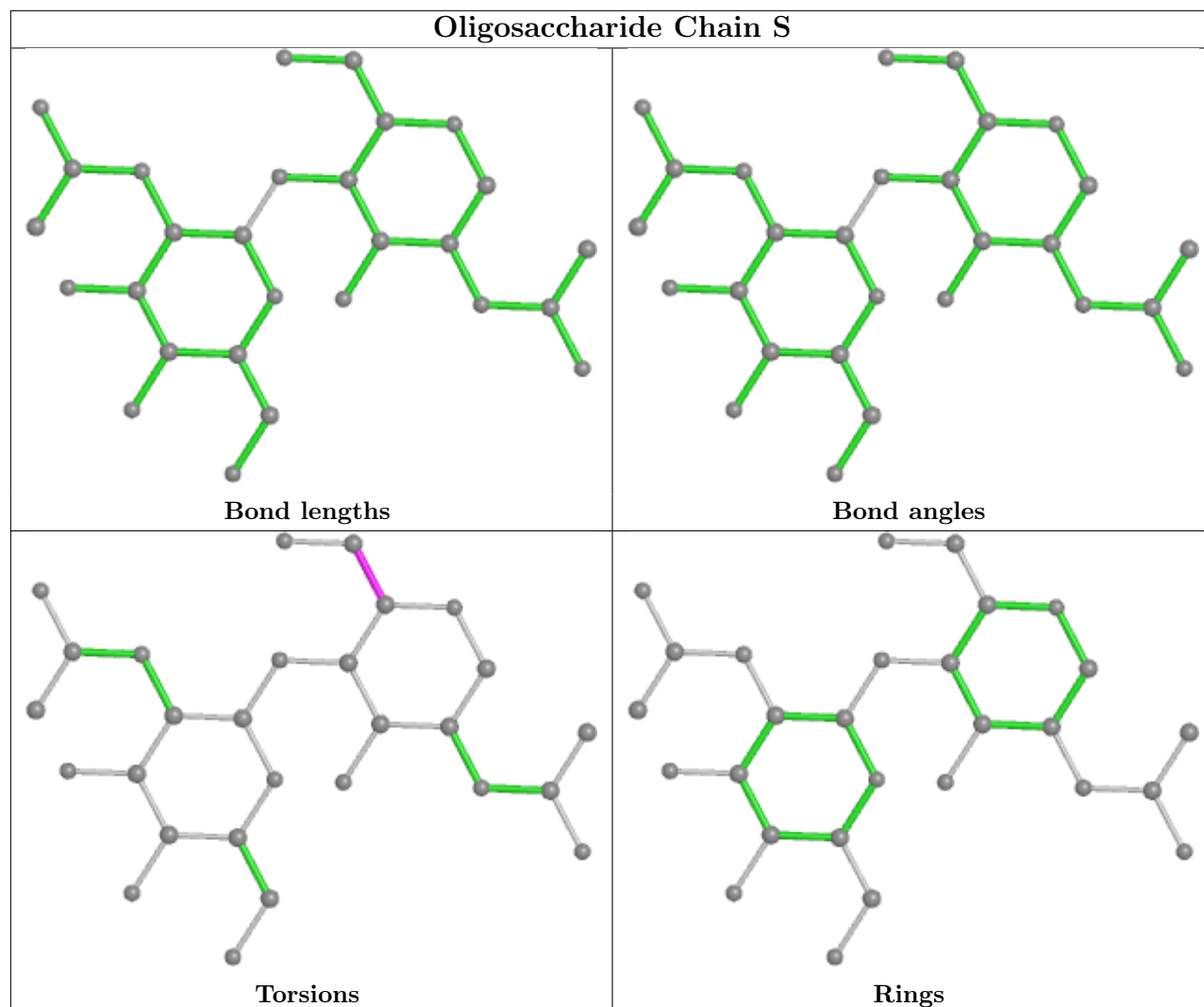


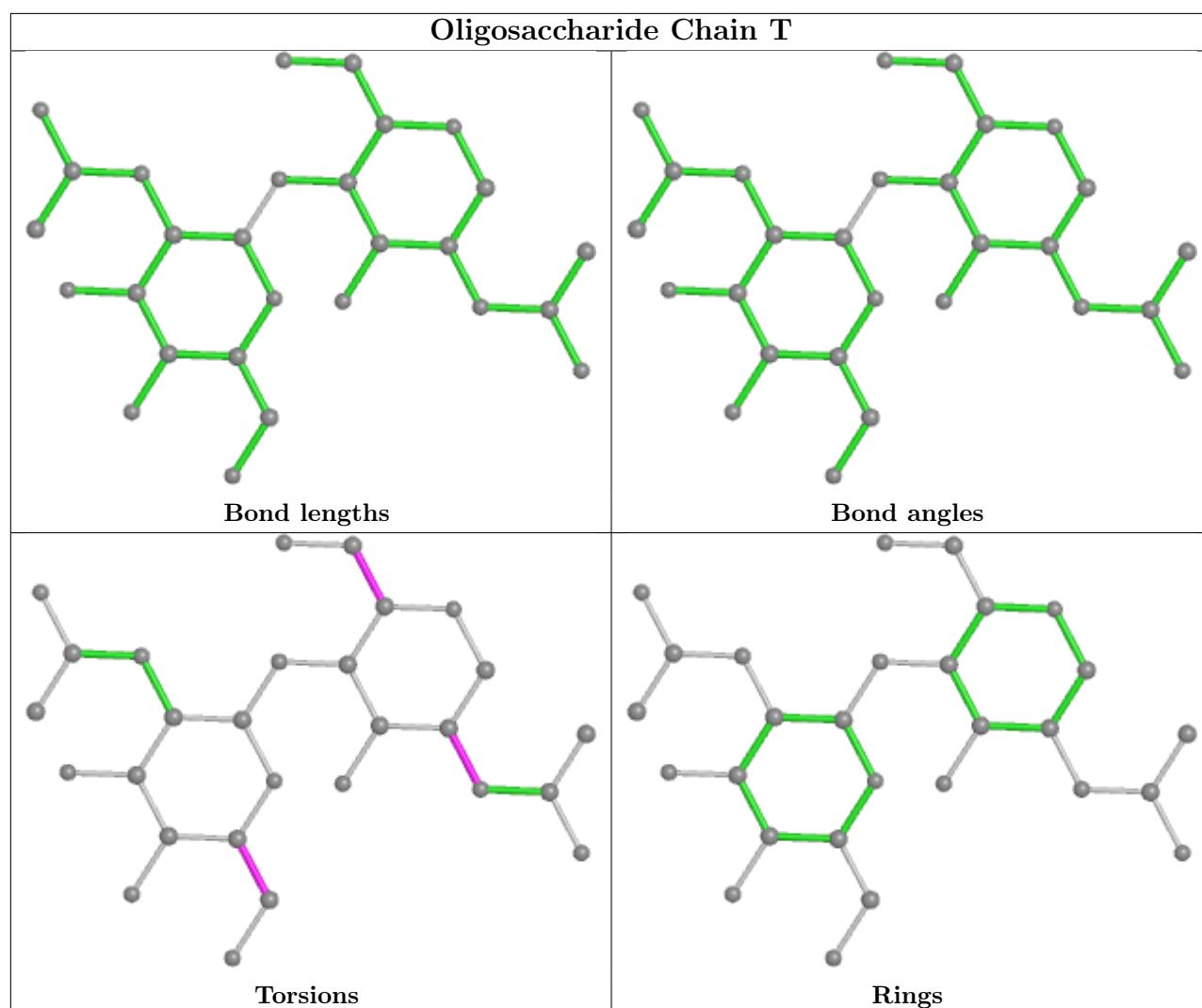


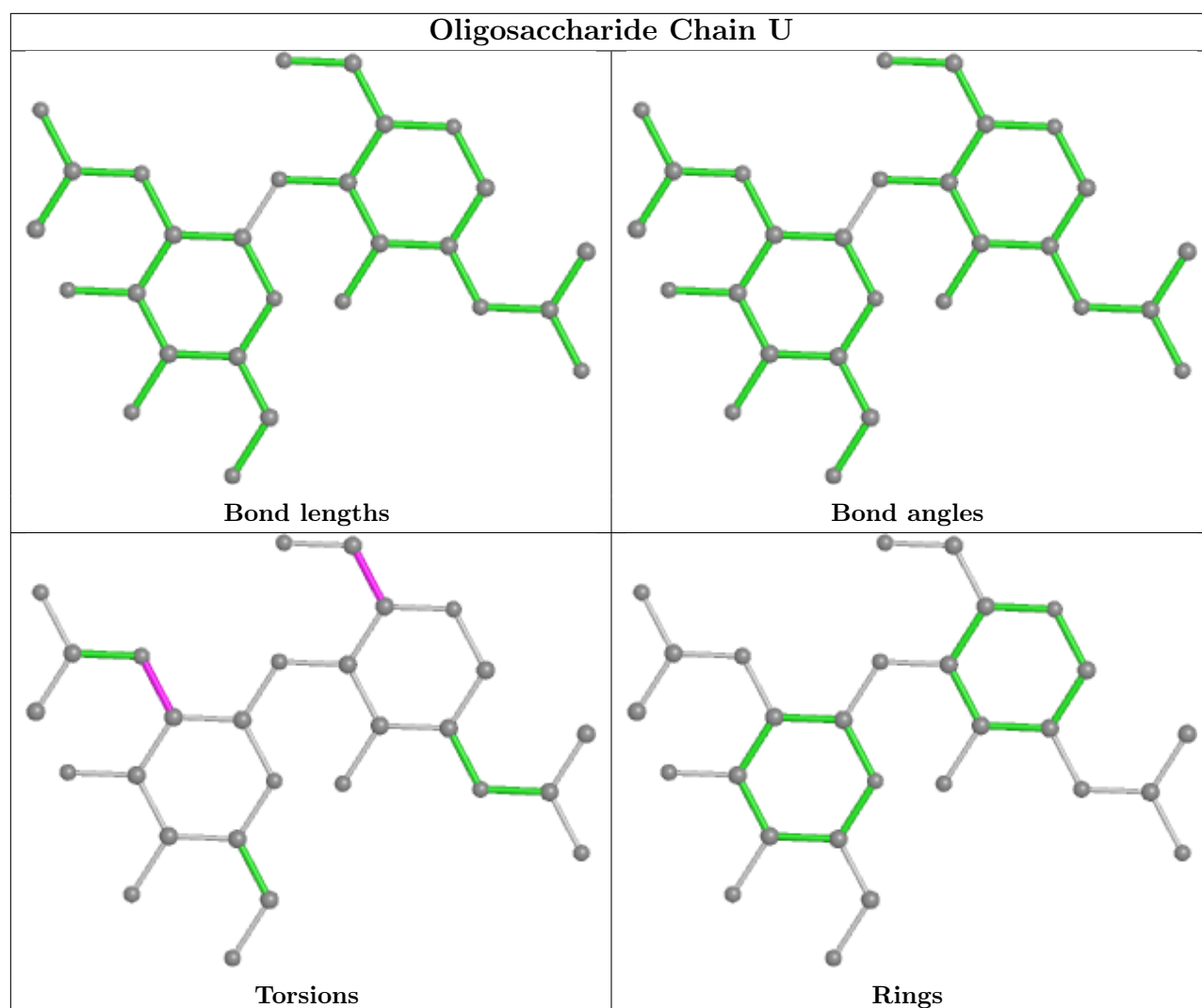


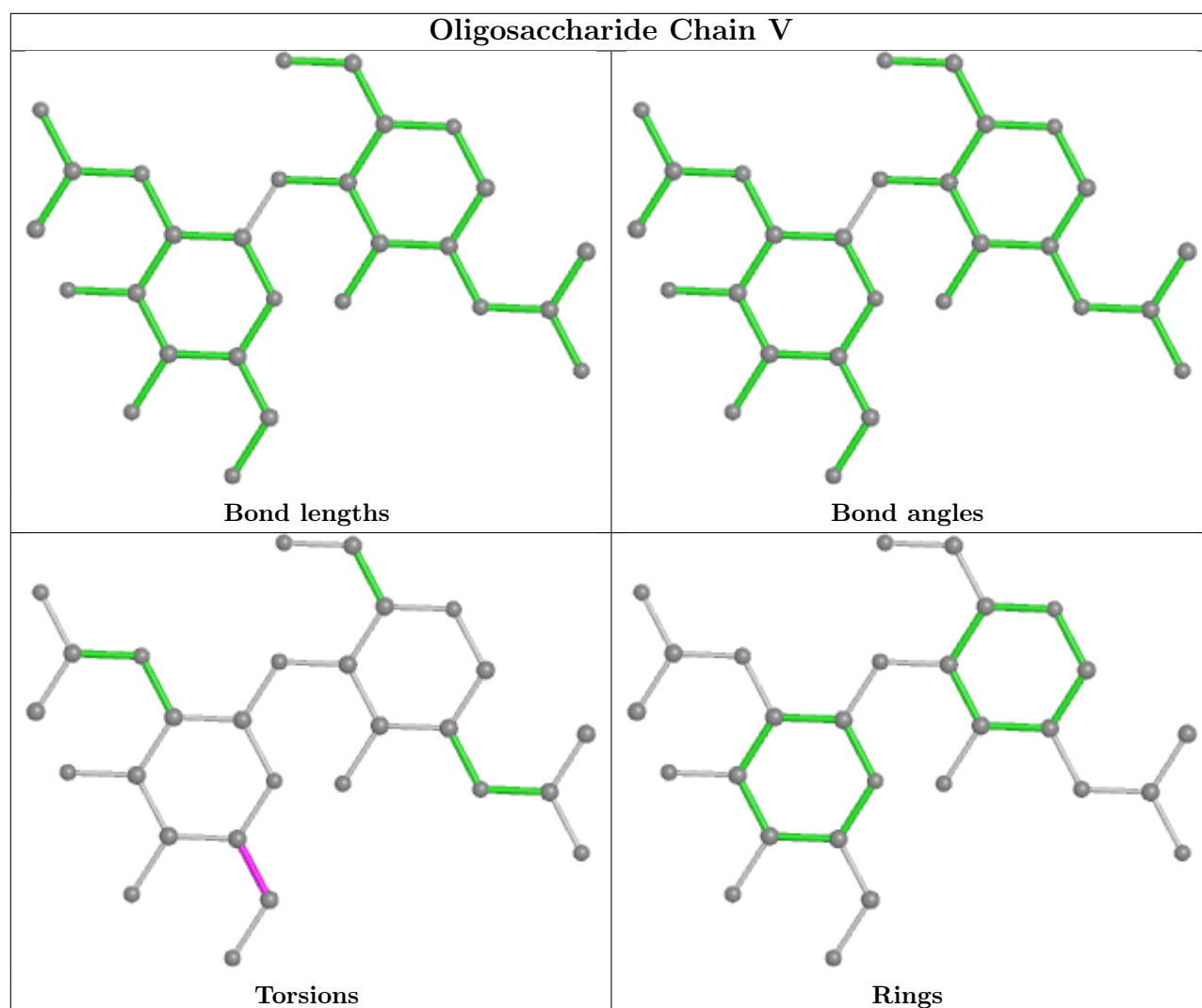


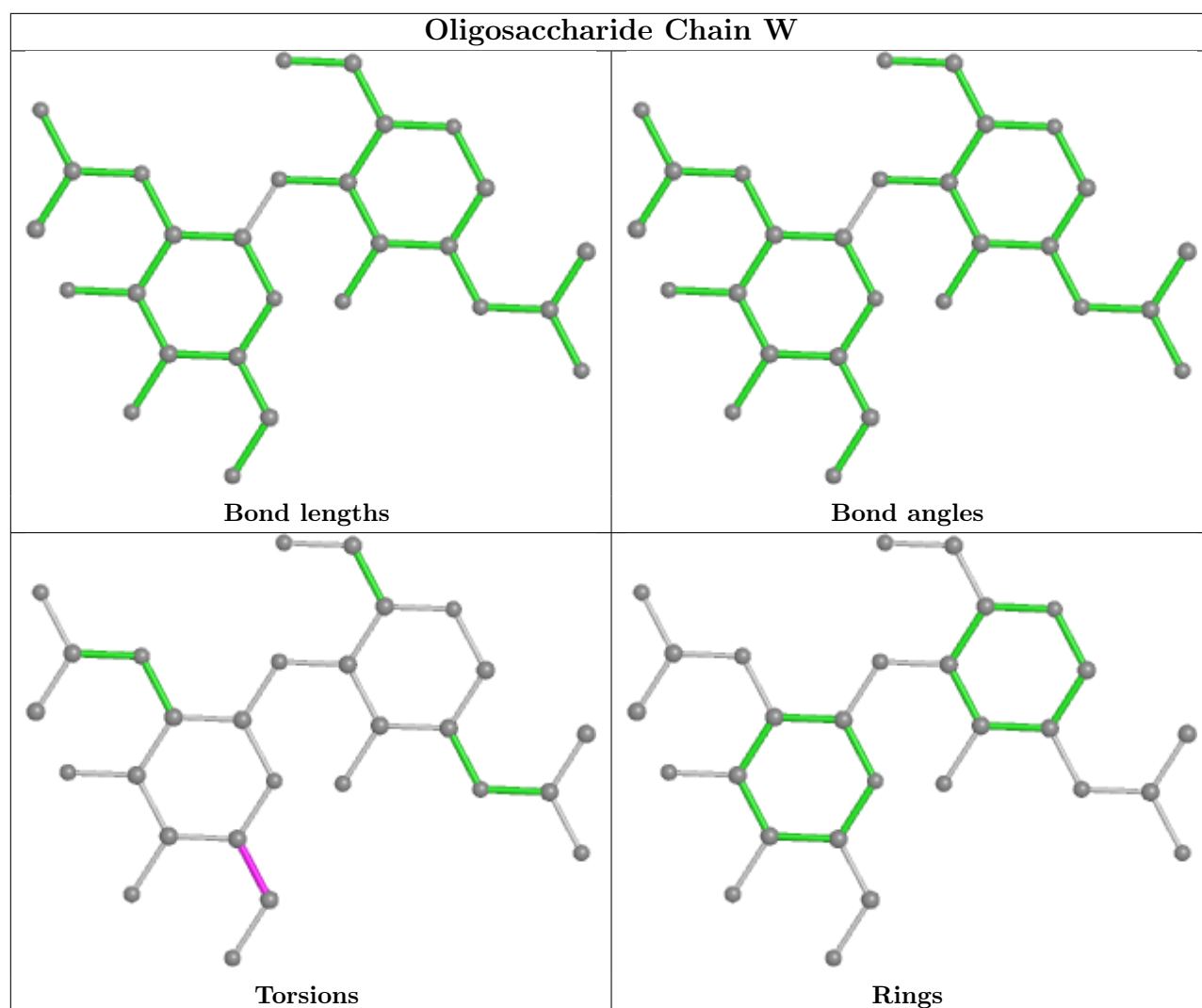


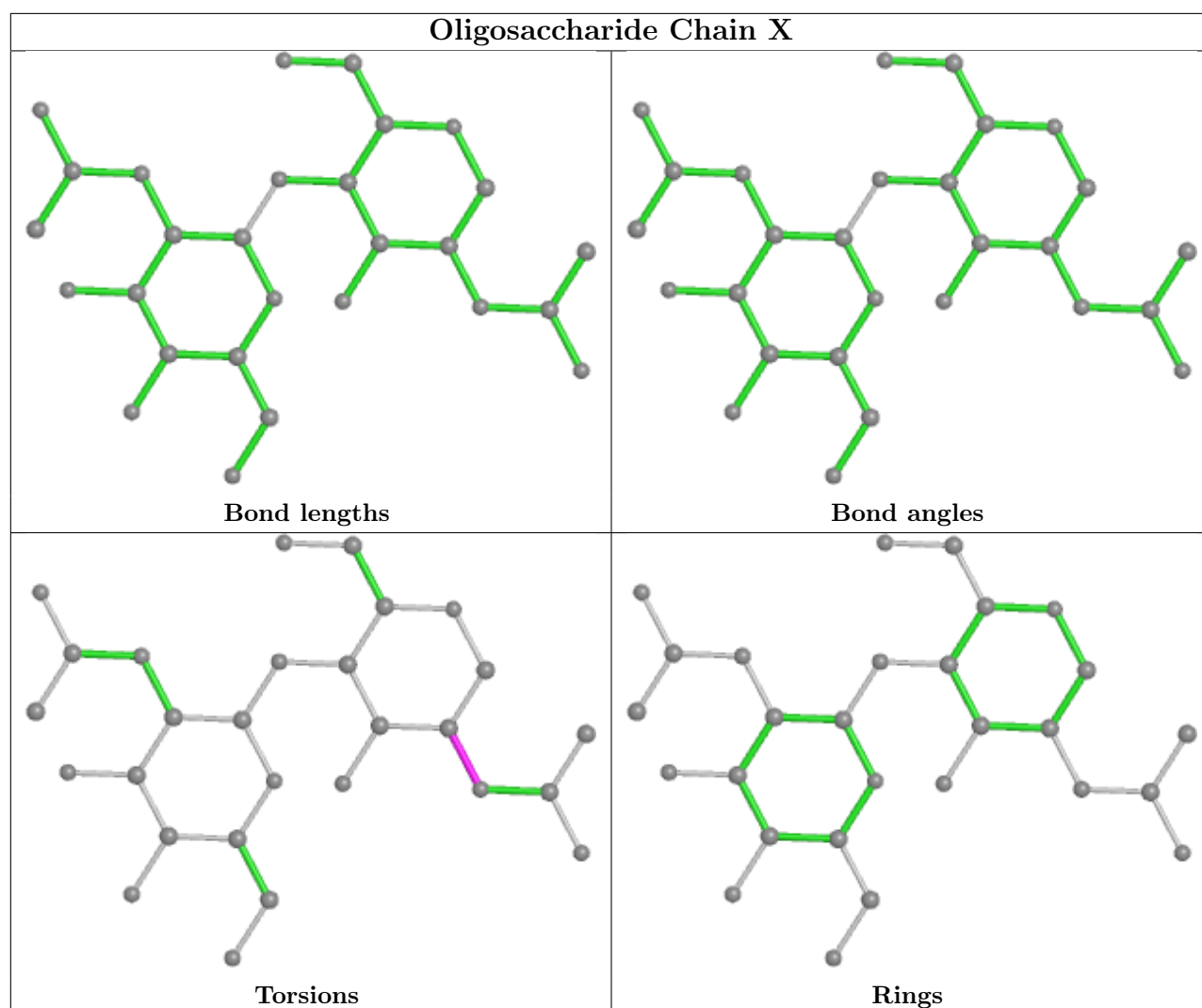


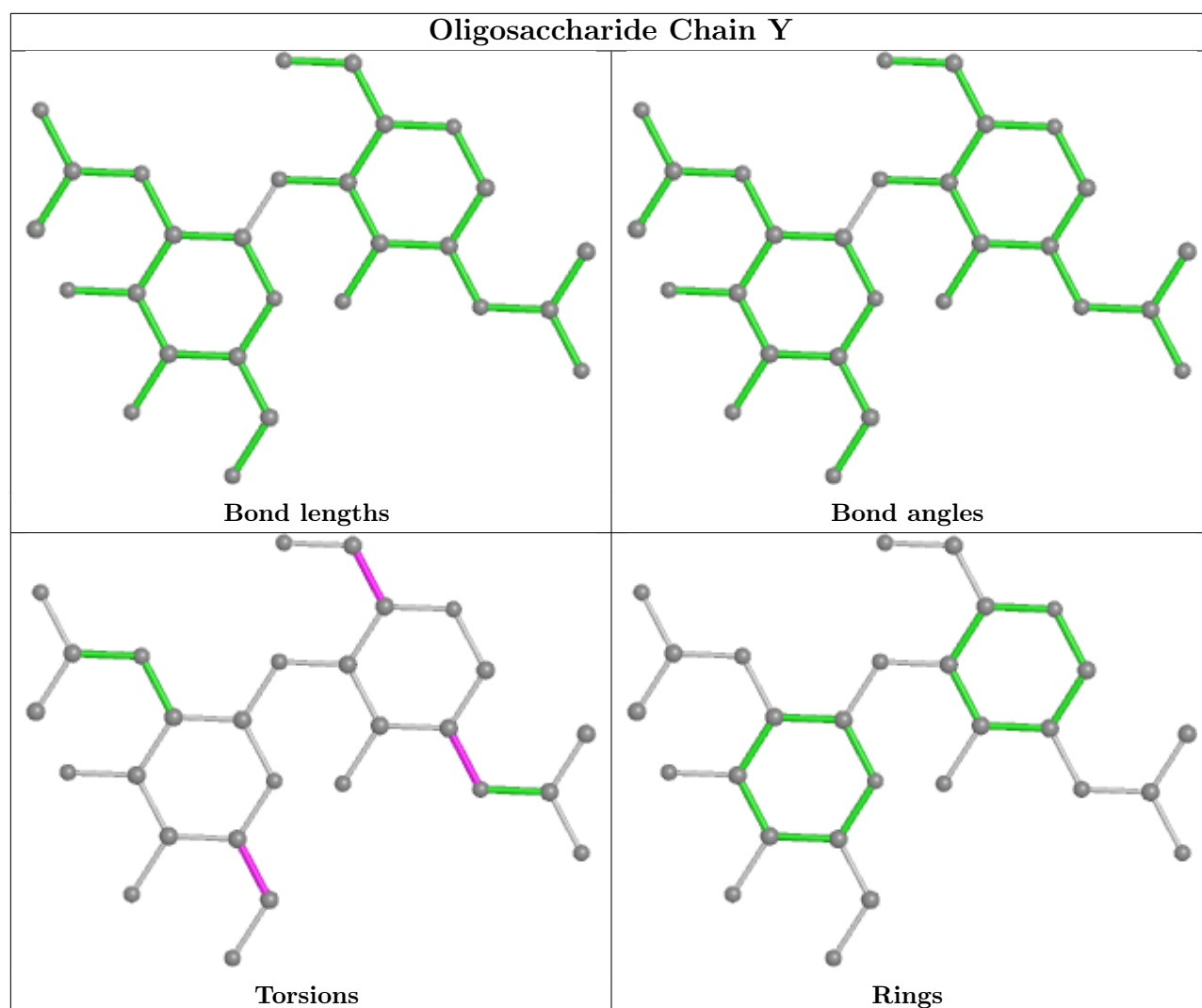


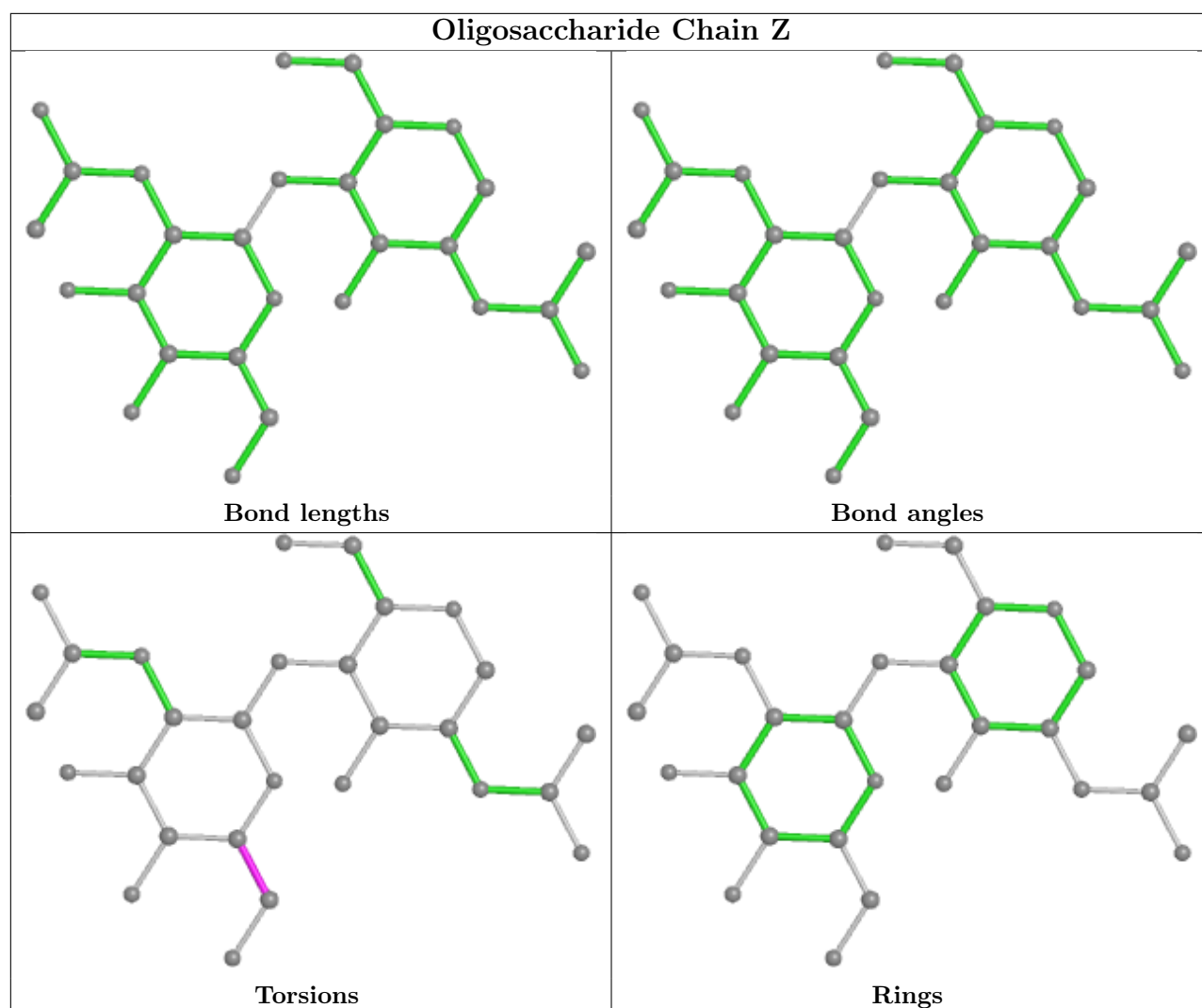


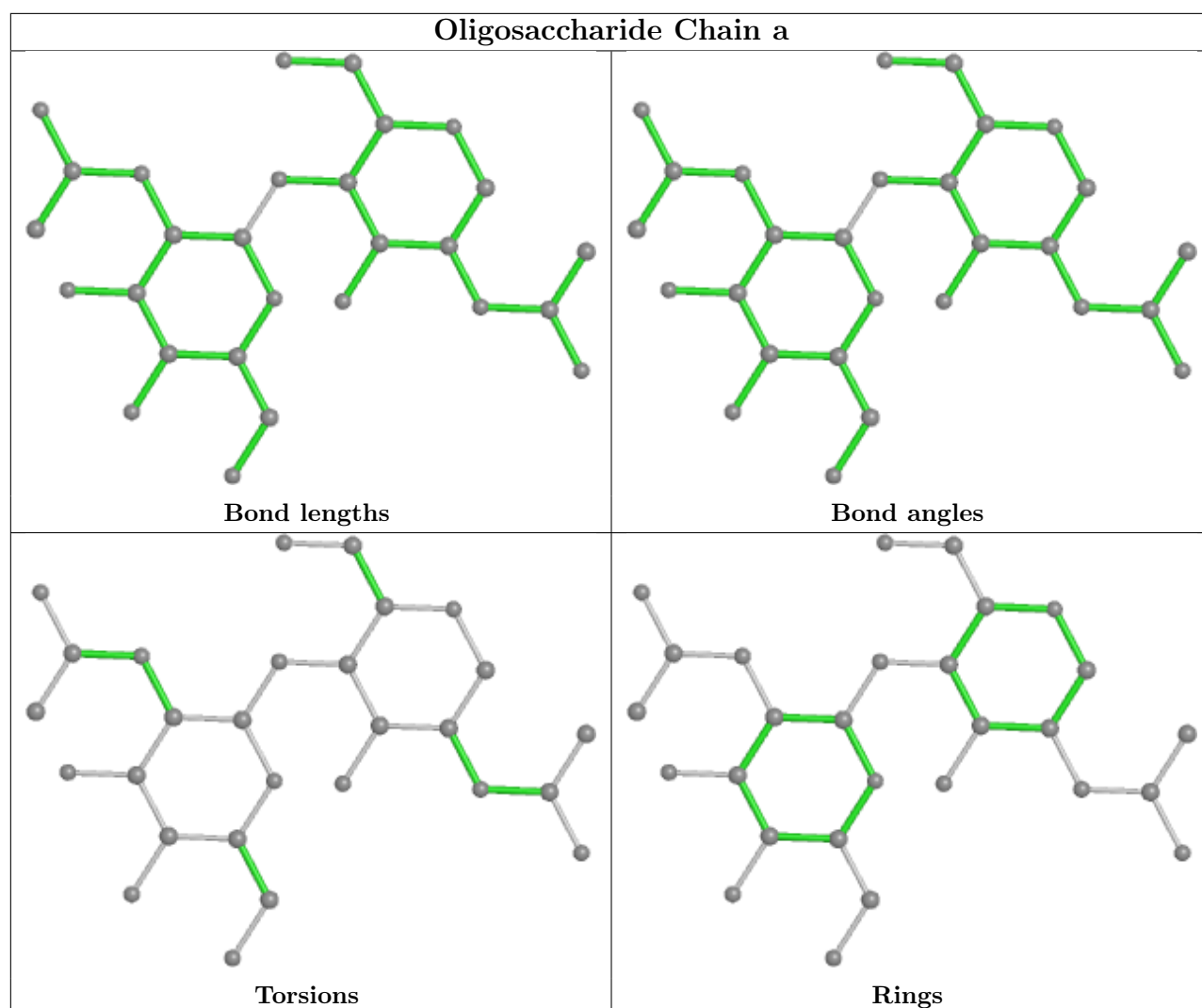


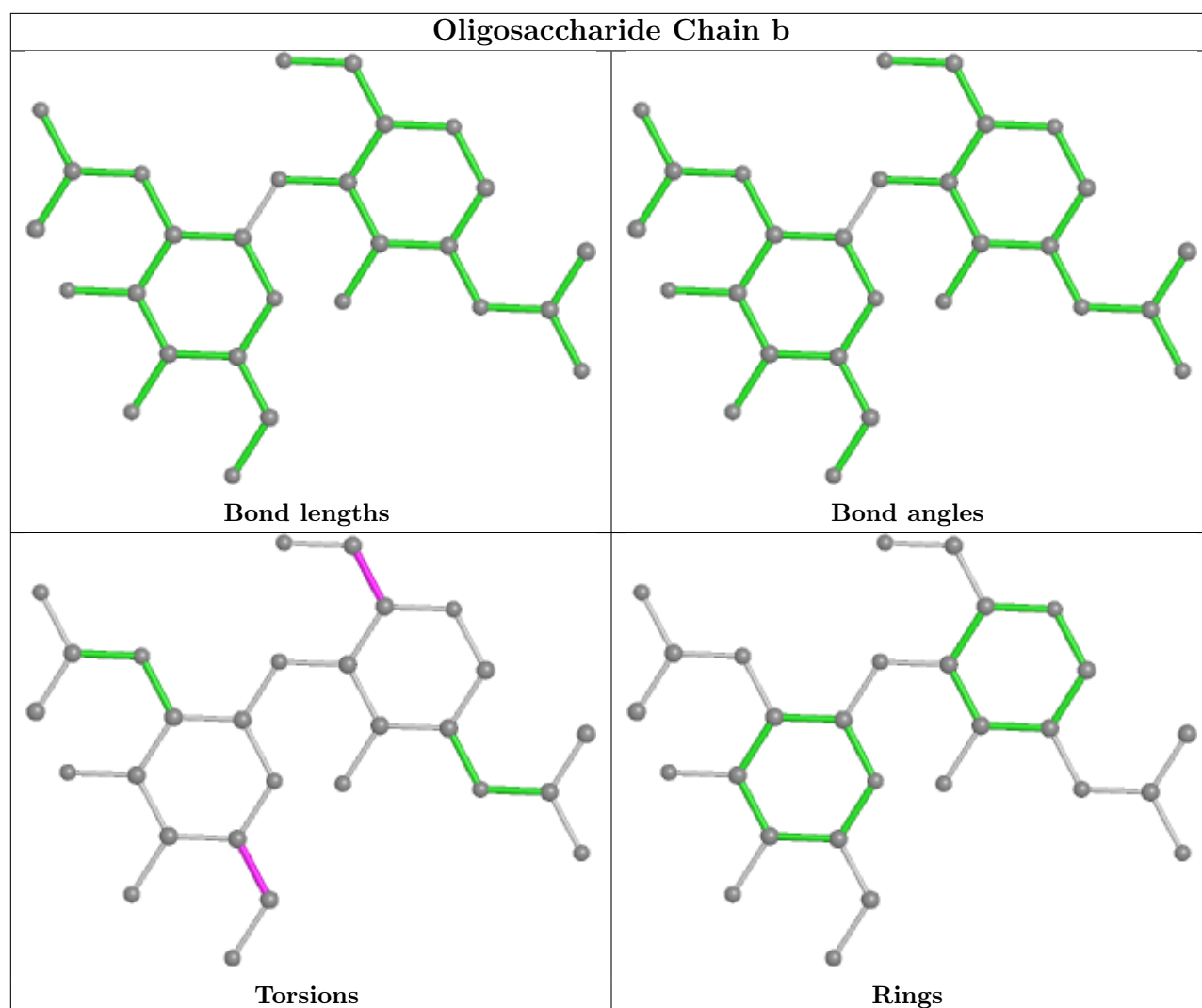


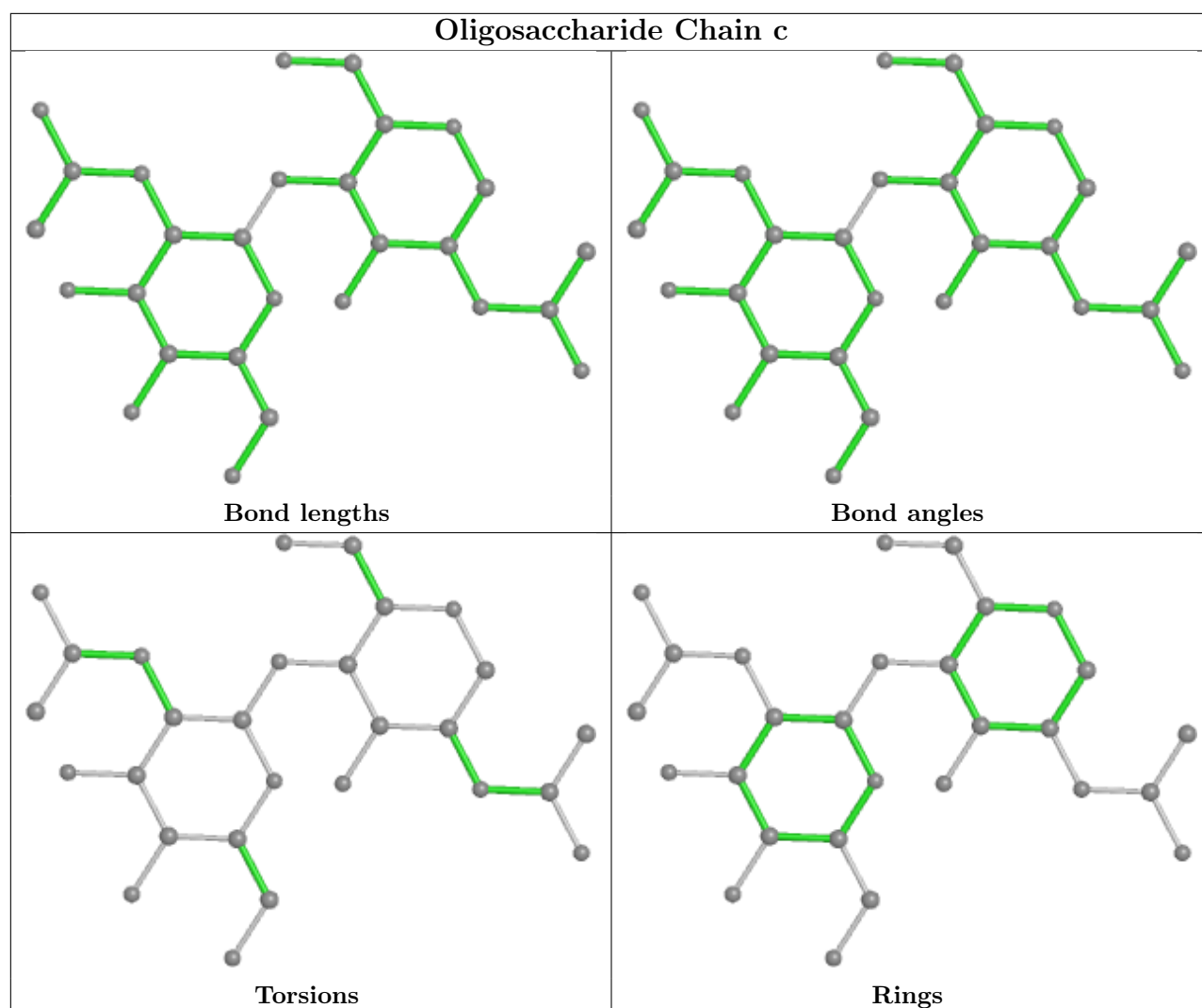


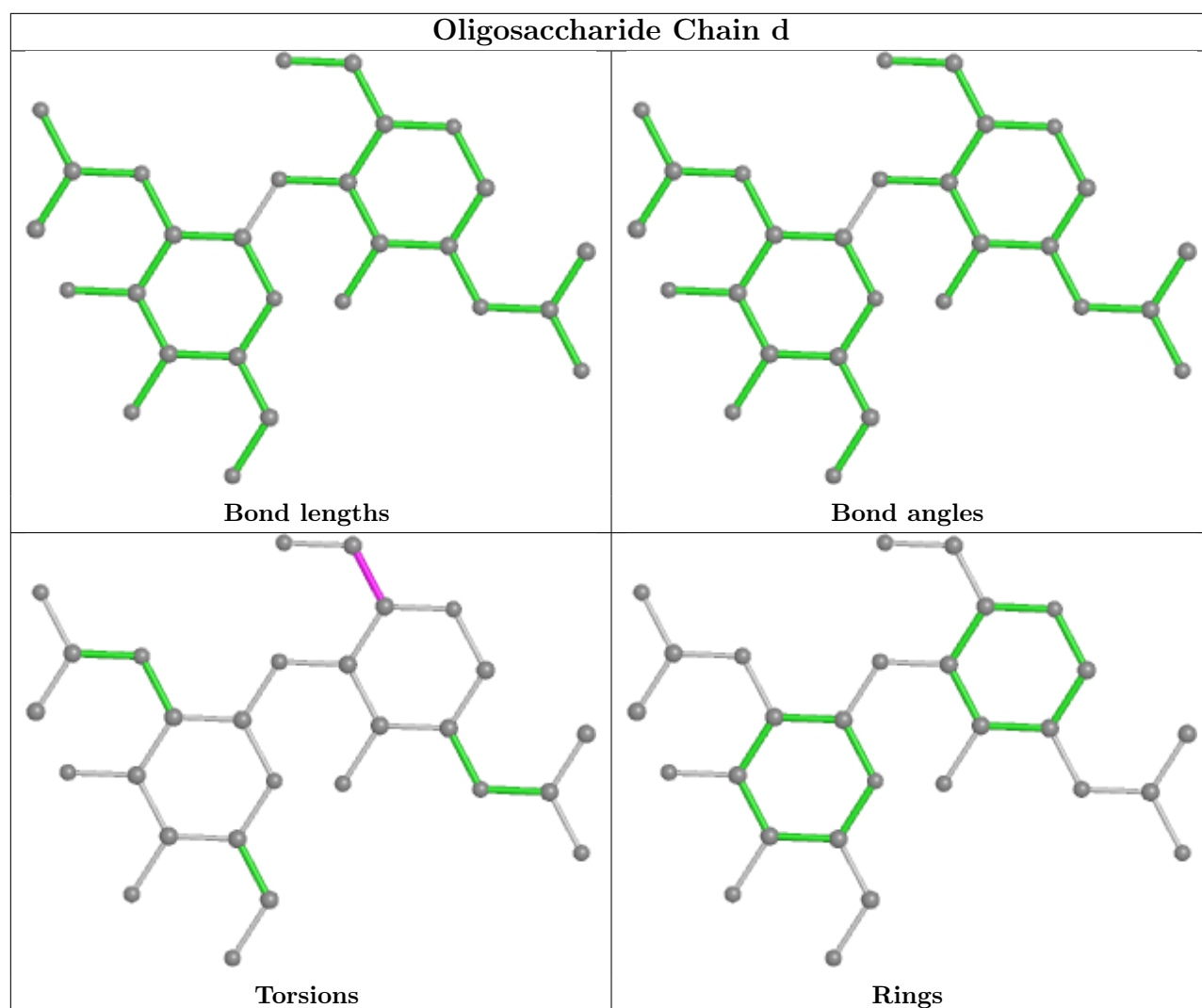


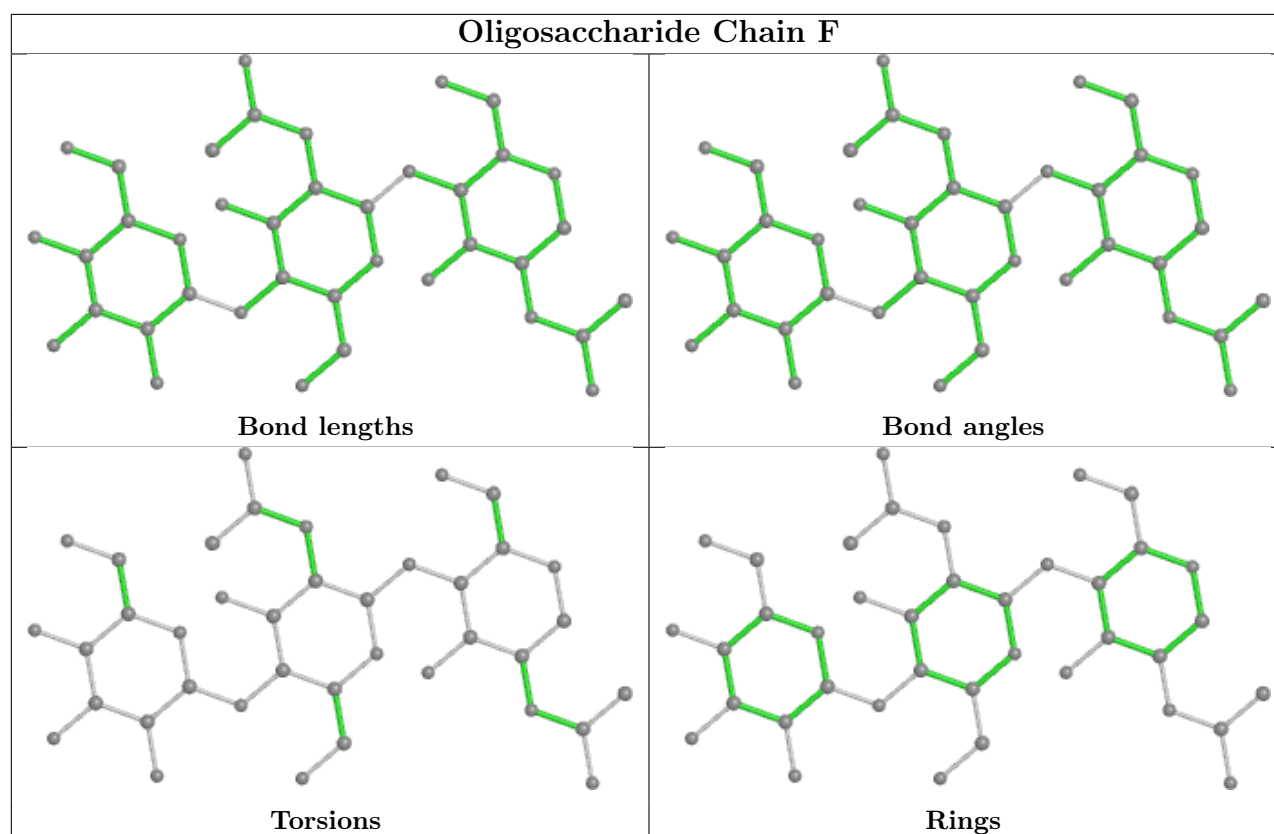












5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	1306	3	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	B	1306	3	14,14,15	0.31	0	17,19,21	0.45	0
6	NAG	A	1302	3	14,14,15	0.26	0	17,19,21	0.46	0
6	NAG	C	1301	3	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	B	1305	3	14,14,15	0.23	0	17,19,21	0.42	0
6	NAG	B	1301	3	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	C	1304	3	14,14,15	0.25	0	17,19,21	0.54	0
6	NAG	A	1304	3	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	A	1306	3	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	A	1303	3	14,14,15	0.22	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	1302	3	14,14,15	0.25	0	17,19,21	0.53	0
6	NAG	A	1305	3	14,14,15	0.25	0	17,19,21	0.55	0
6	NAG	B	1303	3	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	C	1302	3	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	C	1305	3	14,14,15	0.28	0	17,19,21	0.46	0
6	NAG	A	1301	3	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	B	1304	3	14,14,15	0.23	0	17,19,21	0.42	0
6	NAG	C	1303	3	14,14,15	0.25	0	17,19,21	0.54	0
6	NAG	A	1307	3	14,14,15	0.21	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1306	3	-	2/6/23/26	0/1/1/1
6	NAG	B	1306	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1302	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1301	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1305	3	-	1/6/23/26	0/1/1/1
6	NAG	B	1301	3	-	2/6/23/26	0/1/1/1
6	NAG	C	1304	3	-	1/6/23/26	0/1/1/1
6	NAG	A	1304	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1306	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1303	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1302	3	-	3/6/23/26	0/1/1/1
6	NAG	A	1305	3	-	1/6/23/26	0/1/1/1
6	NAG	B	1303	3	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	3	-	2/6/23/26	0/1/1/1
6	NAG	C	1305	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1304	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1303	3	-	3/6/23/26	0/1/1/1
6	NAG	A	1307	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

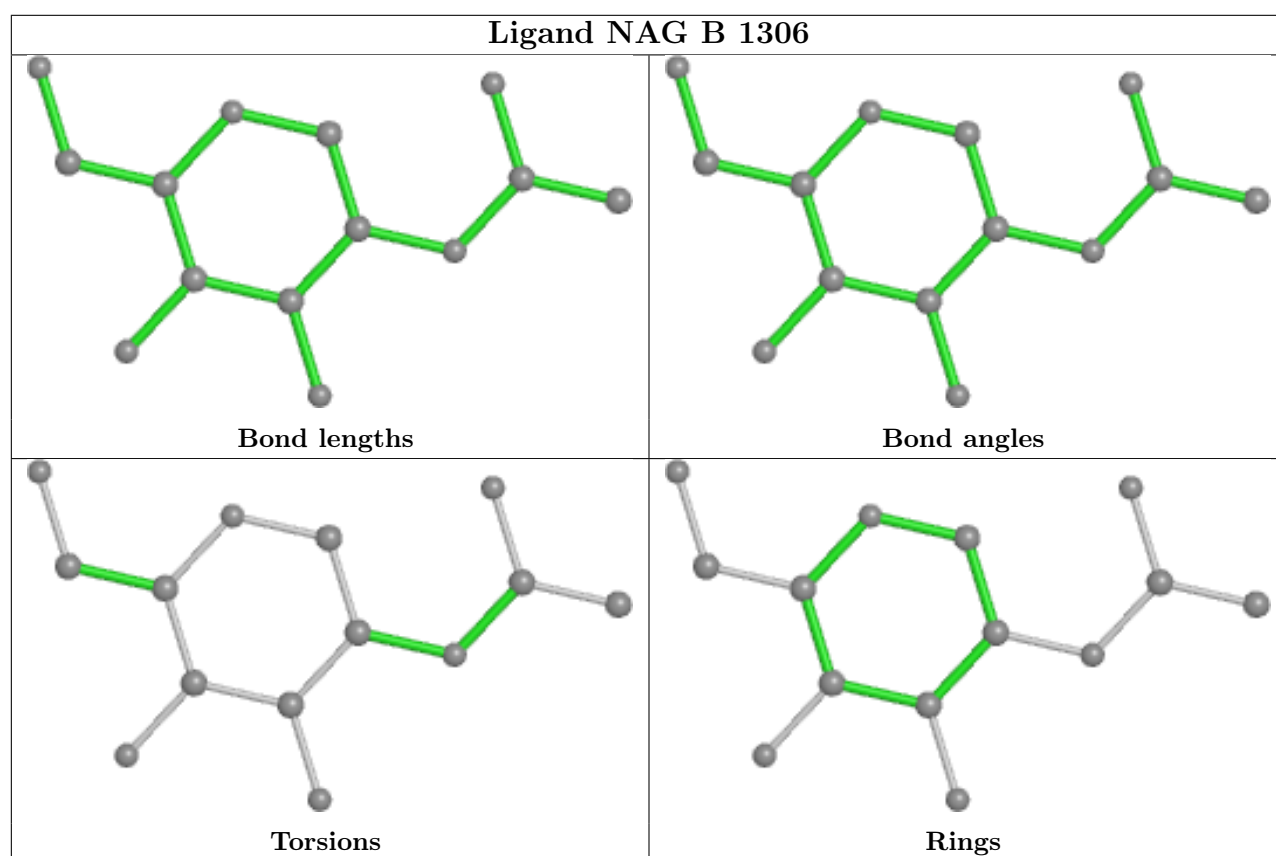
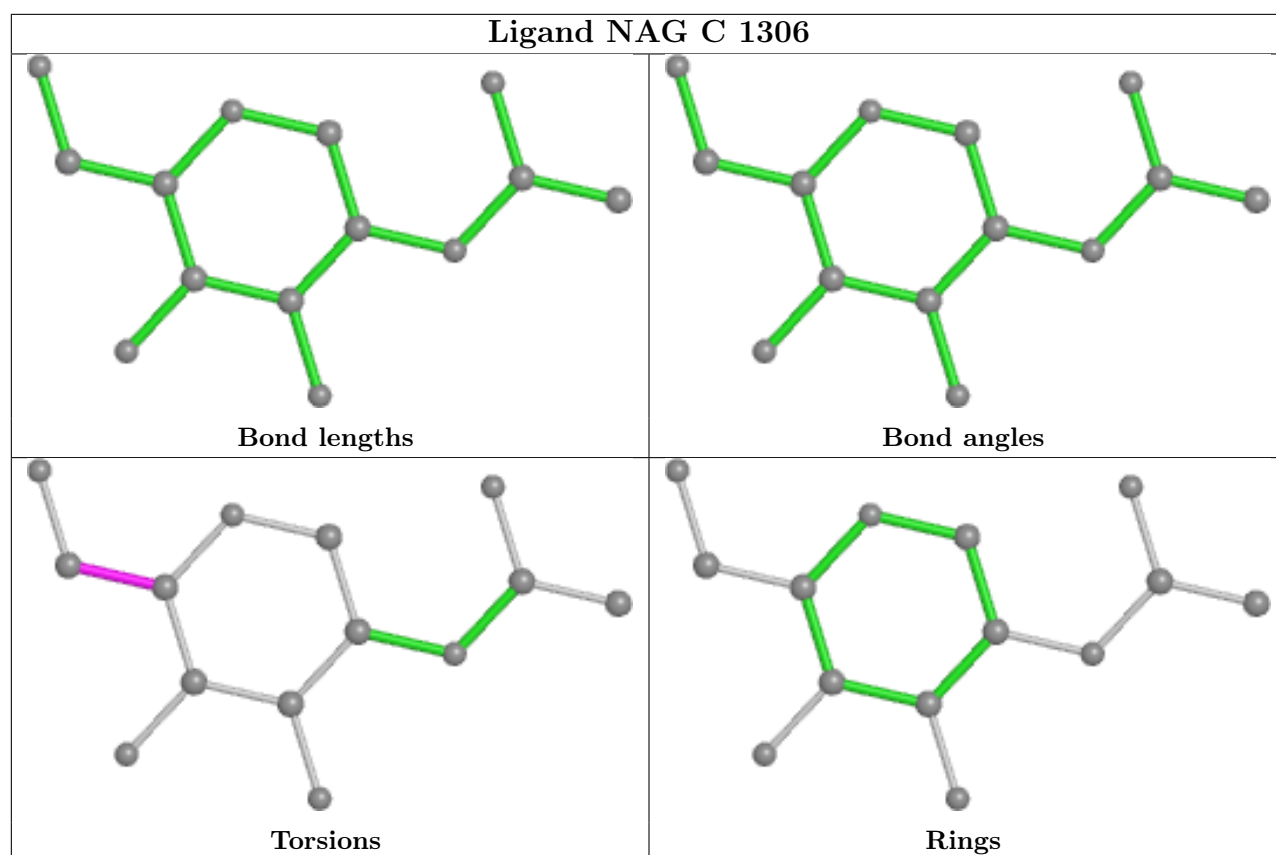
Mol	Chain	Res	Type	Atoms
6	B	1301	NAG	O5-C5-C6-O6
6	A	1307	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	C	1306	NAG	O5-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6
6	C	1306	NAG	C4-C5-C6-O6
6	A	1307	NAG	C4-C5-C6-O6
6	C	1302	NAG	C4-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6
6	C	1302	NAG	O5-C5-C6-O6
6	B	1305	NAG	O5-C5-C6-O6
6	B	1303	NAG	C4-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6
6	C	1305	NAG	C4-C5-C6-O6
6	C	1305	NAG	O5-C5-C6-O6
6	A	1304	NAG	C4-C5-C6-O6
6	C	1303	NAG	C3-C2-N2-C7
6	C	1304	NAG	C3-C2-N2-C7
6	B	1302	NAG	C3-C2-N2-C7
6	A	1305	NAG	C3-C2-N2-C7
6	A	1304	NAG	O5-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6

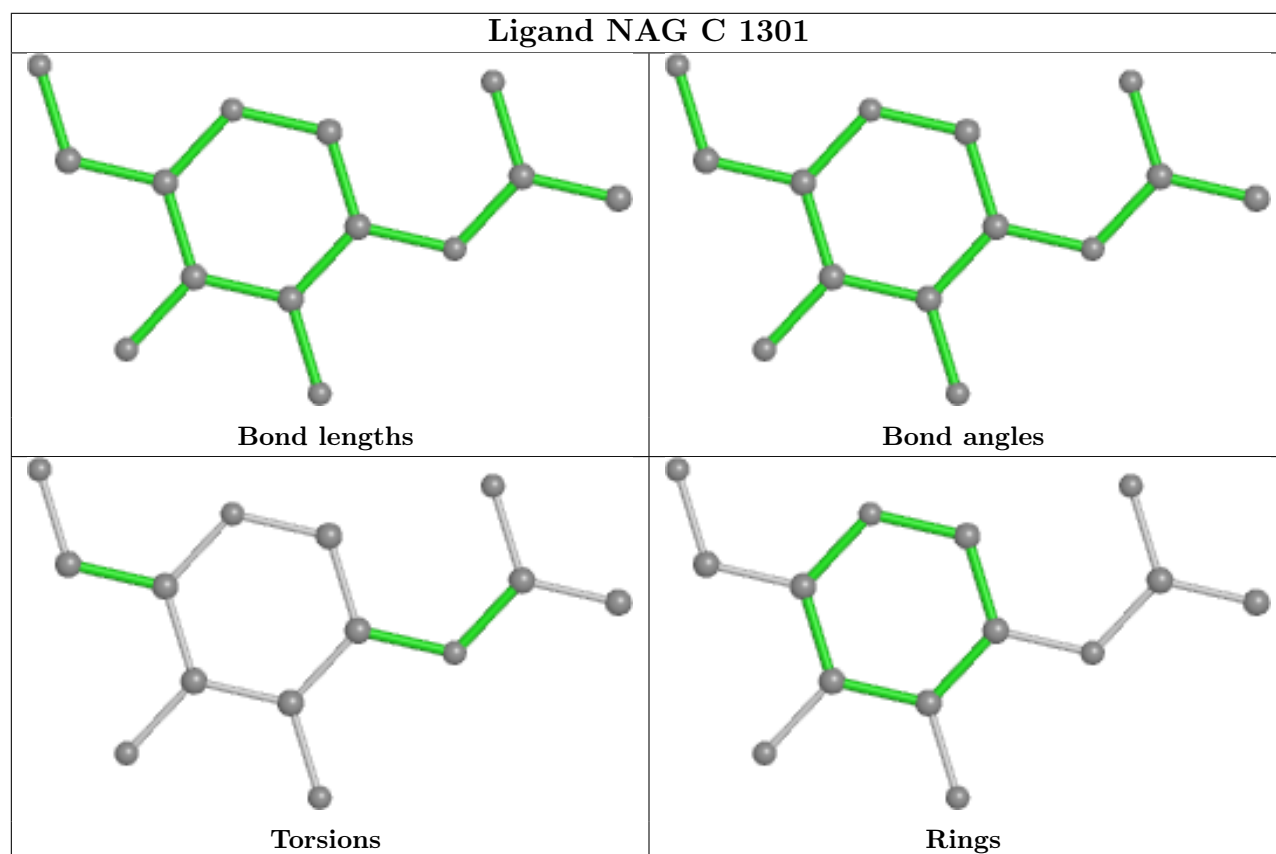
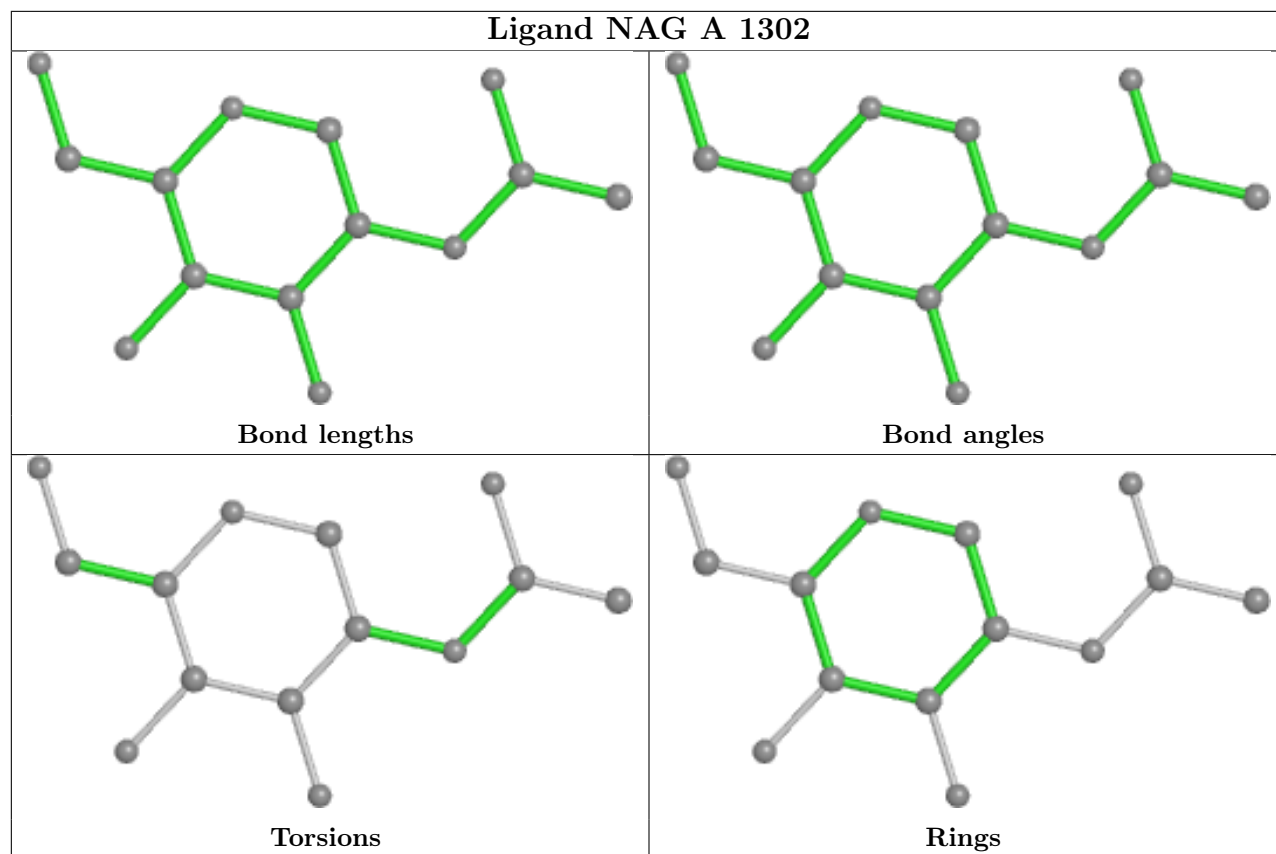
There are no ring outliers.

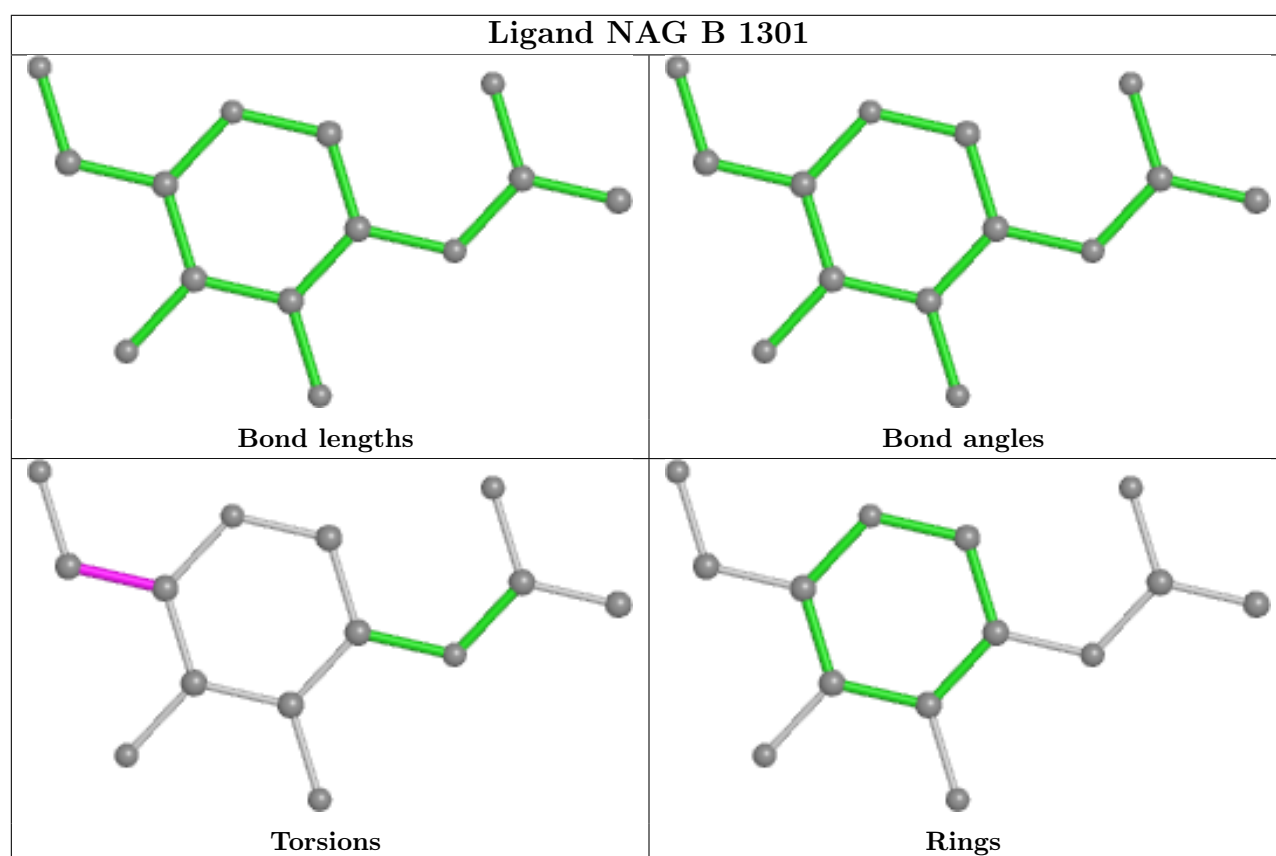
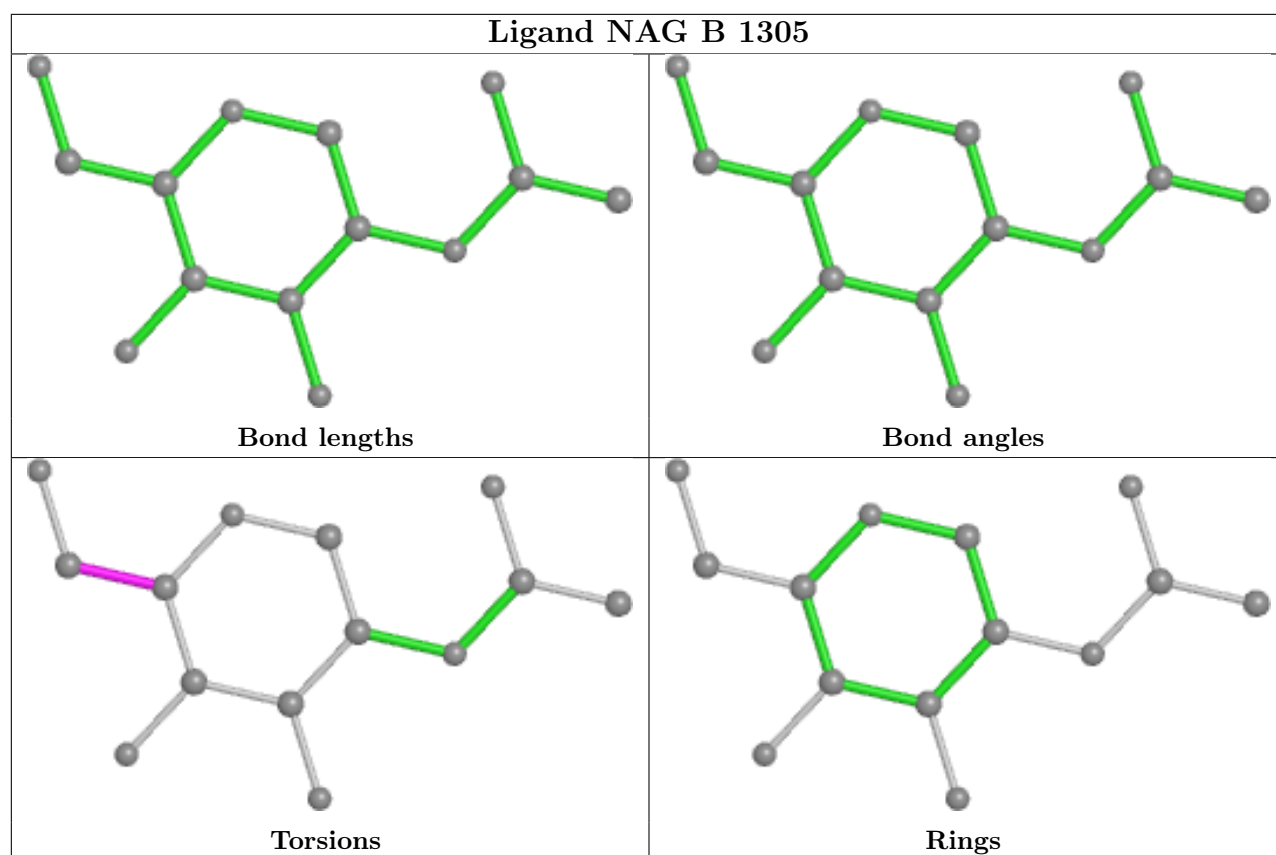
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1301	NAG	1	0

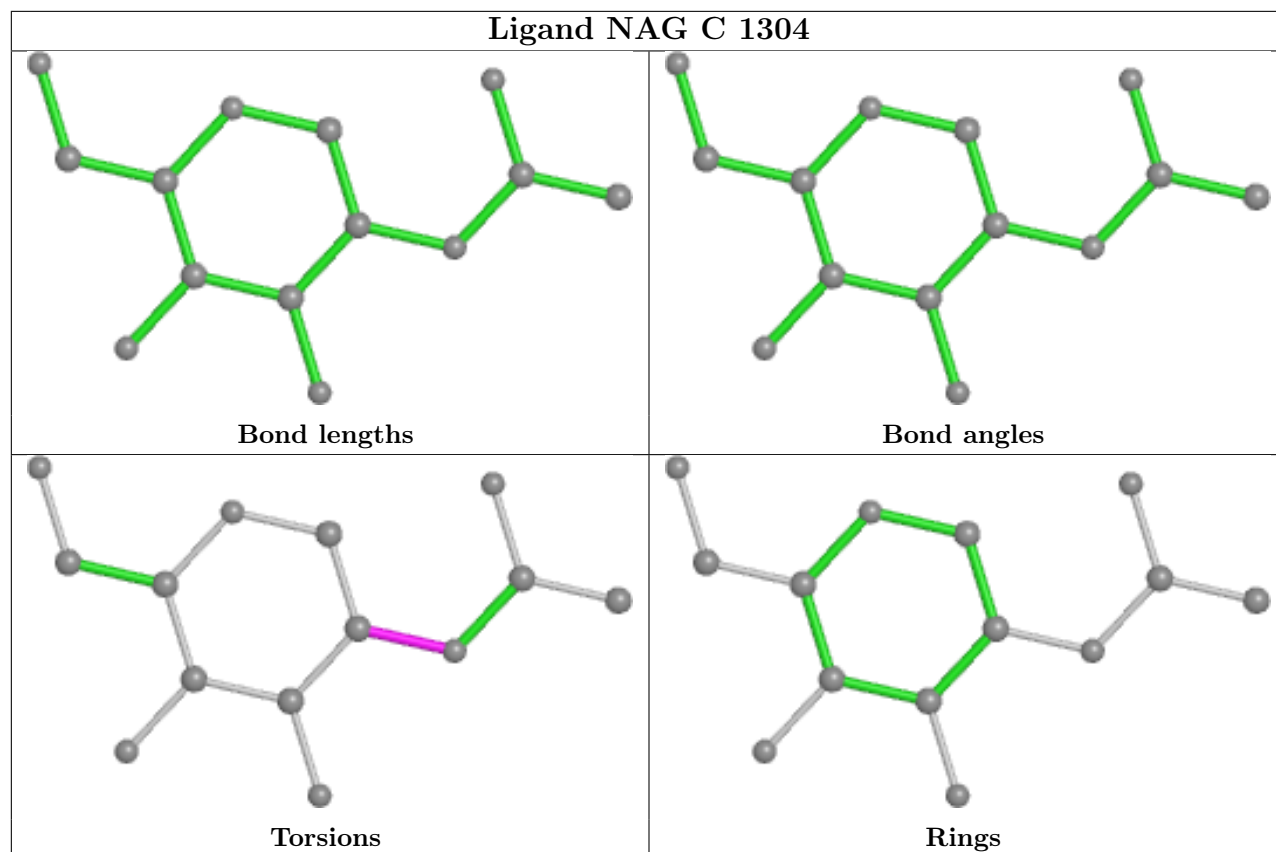
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



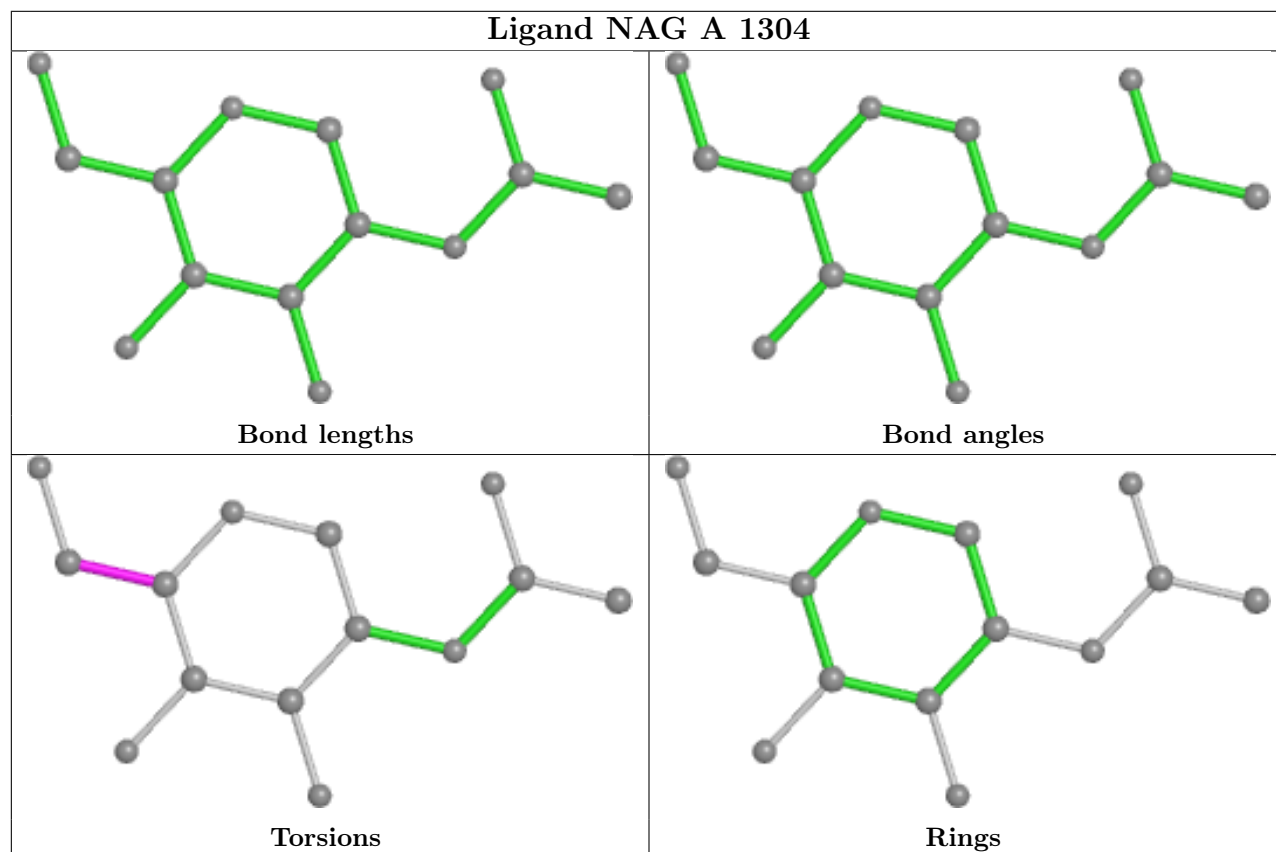


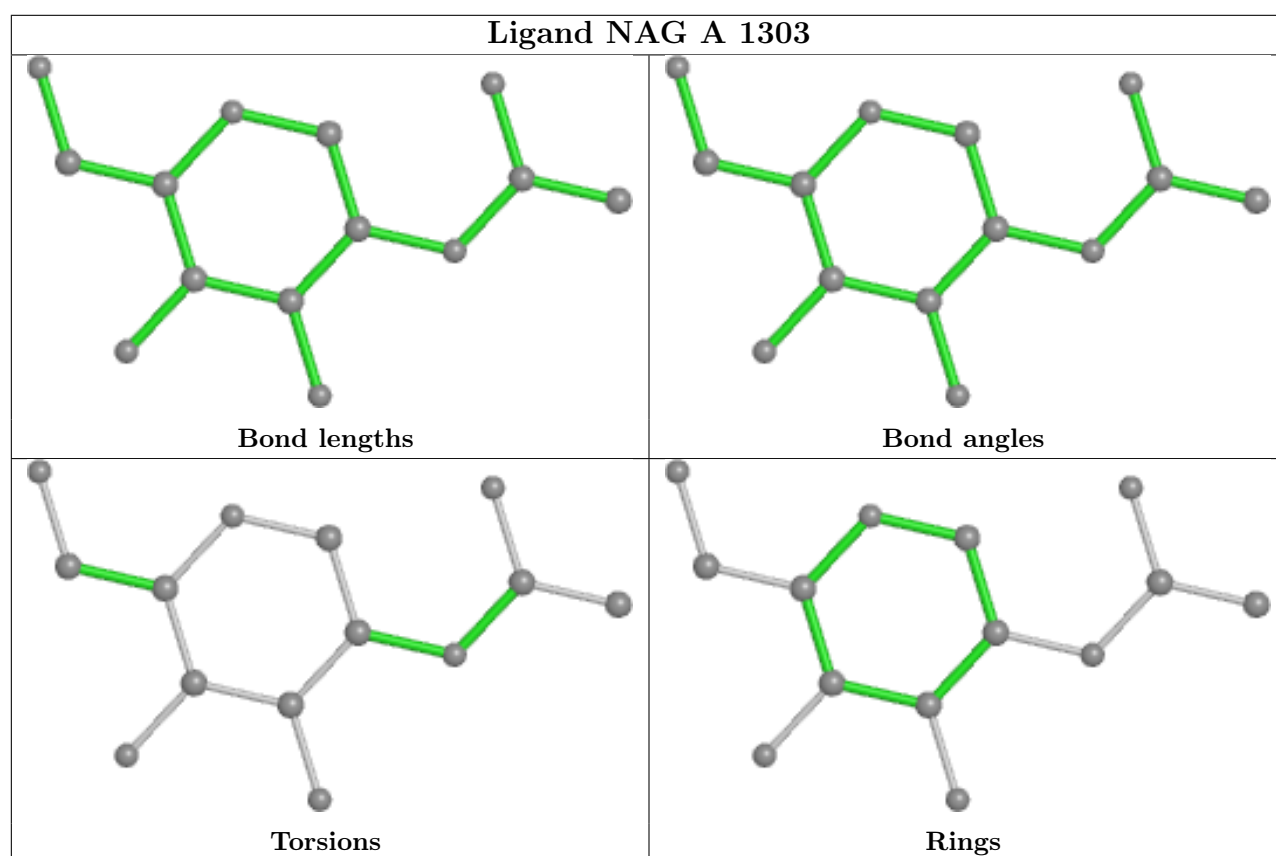
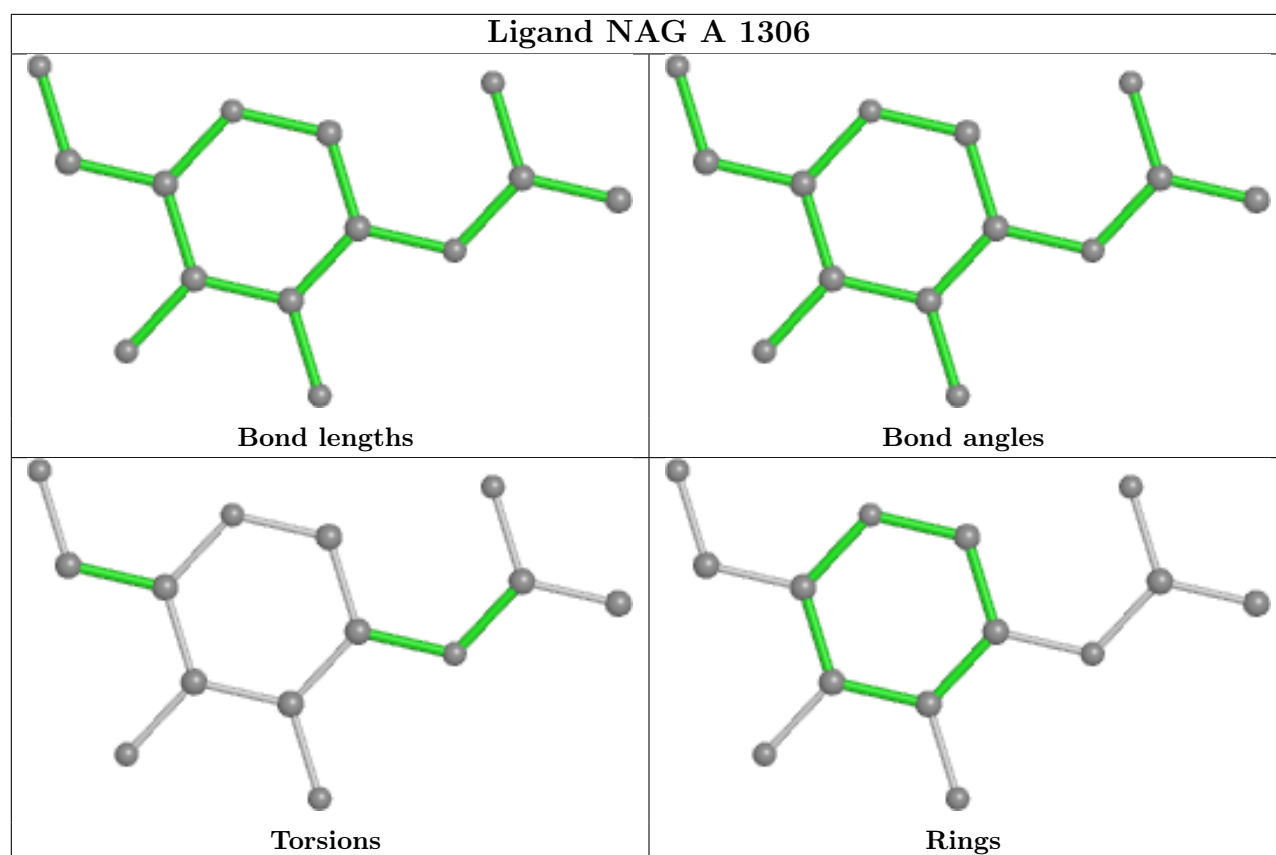


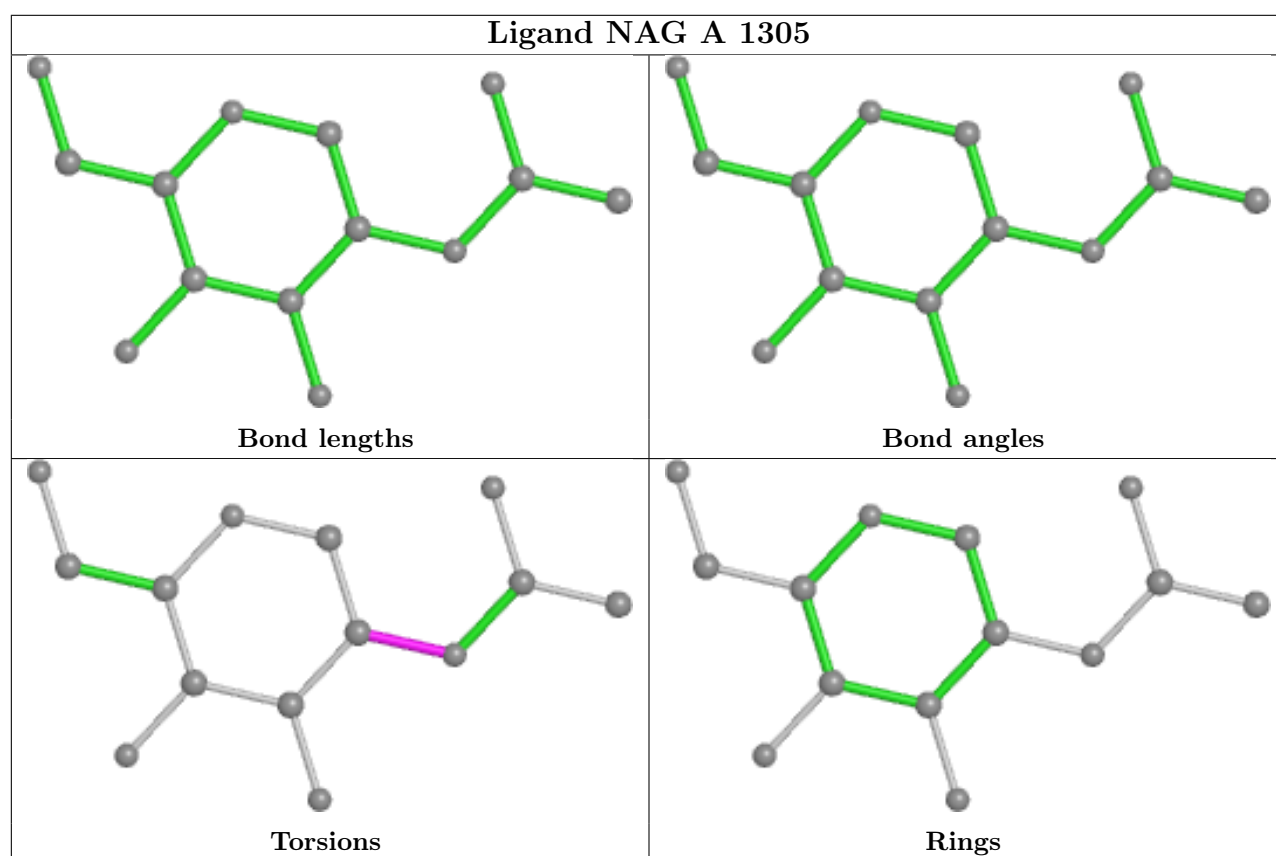
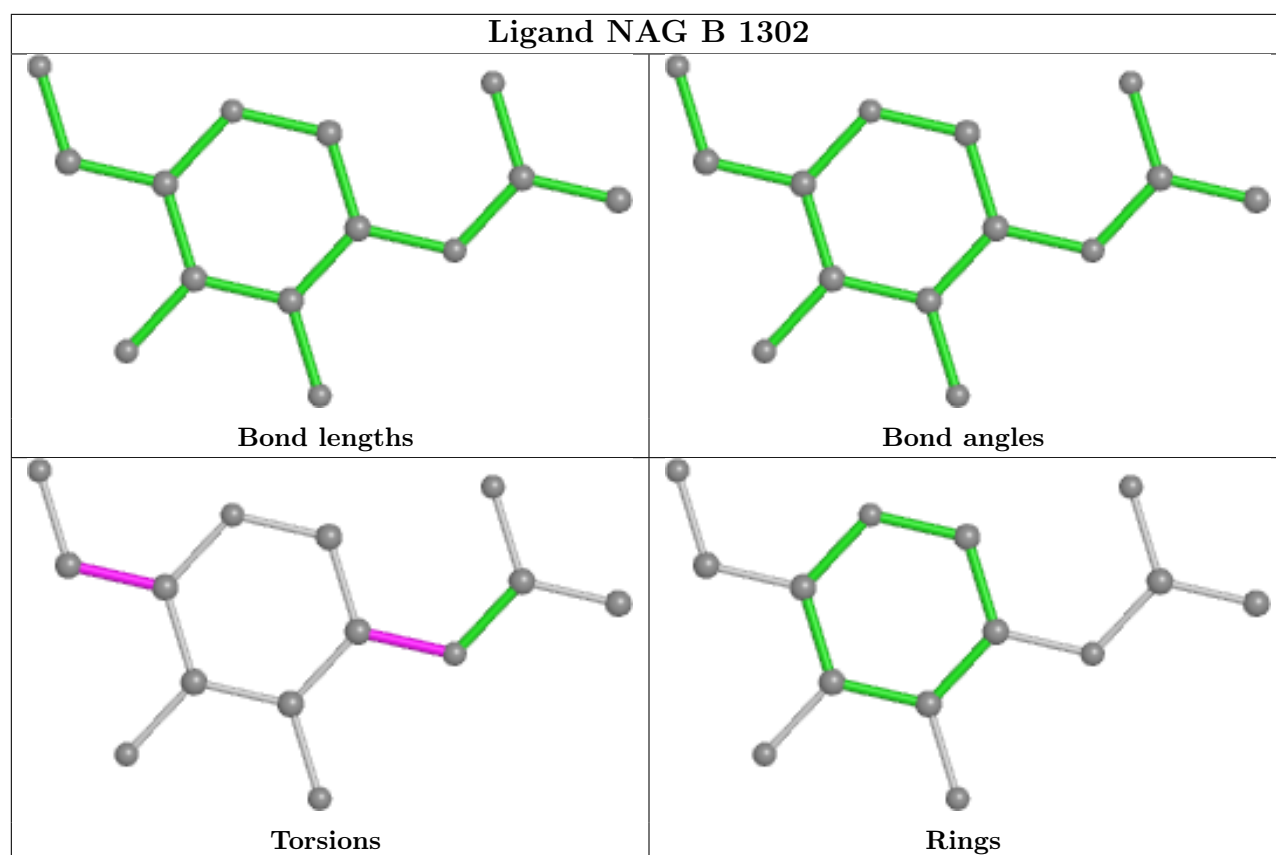
Ligand NAG C 1304

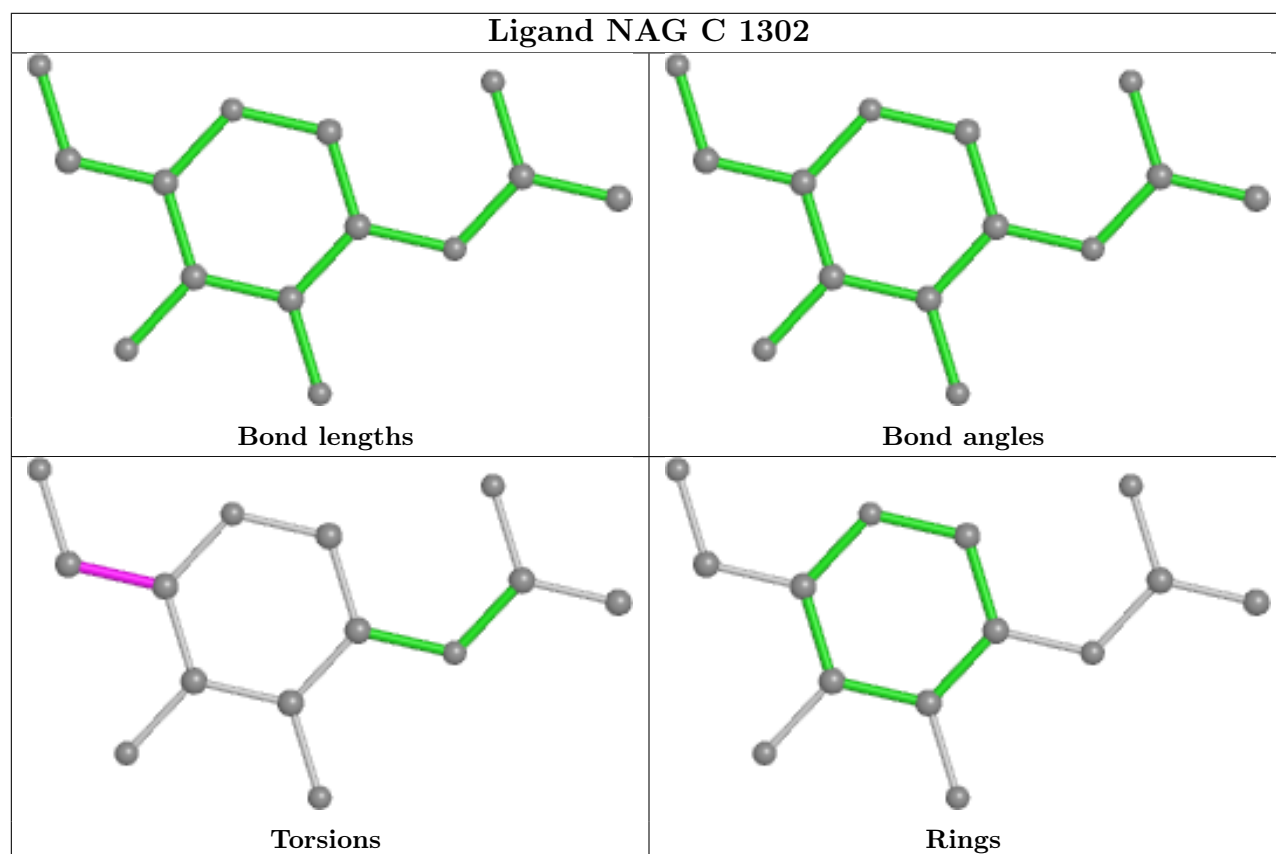
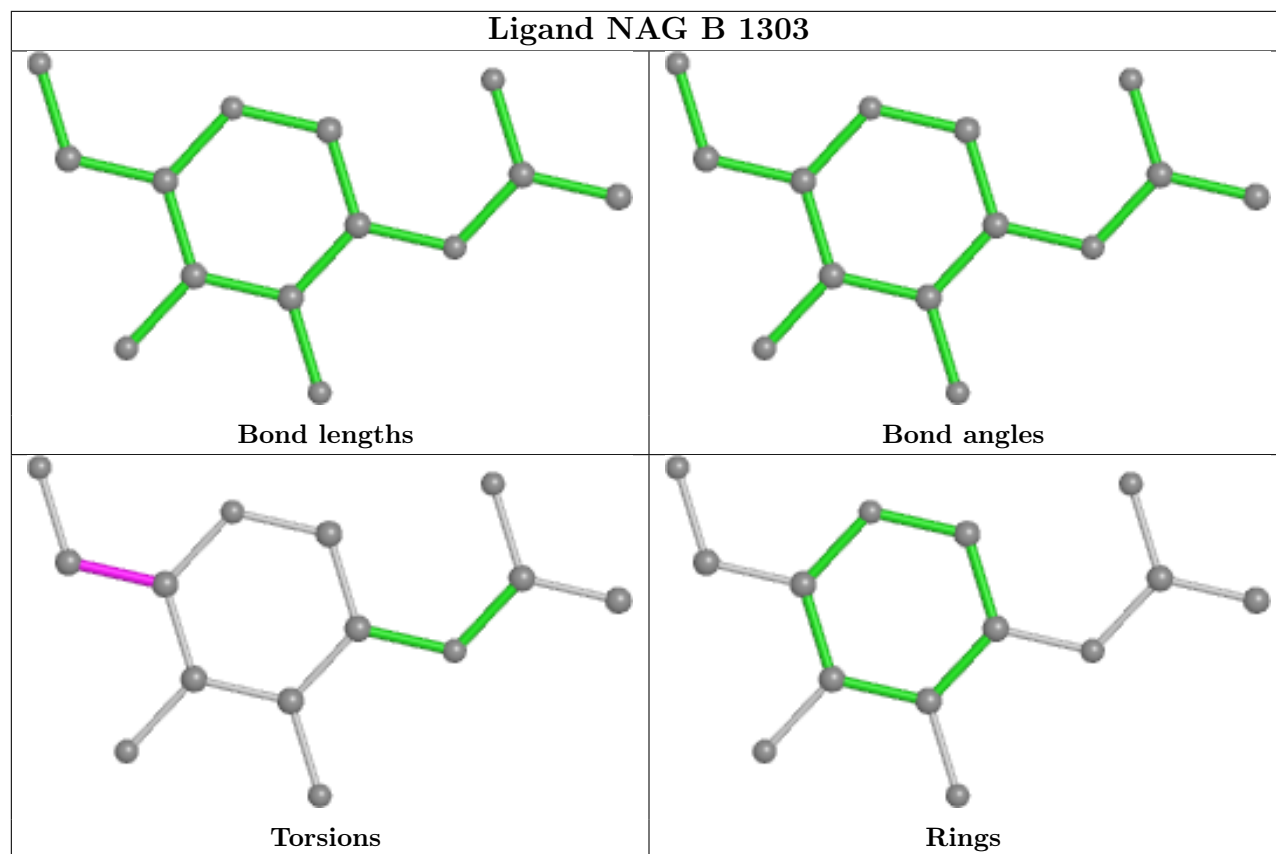


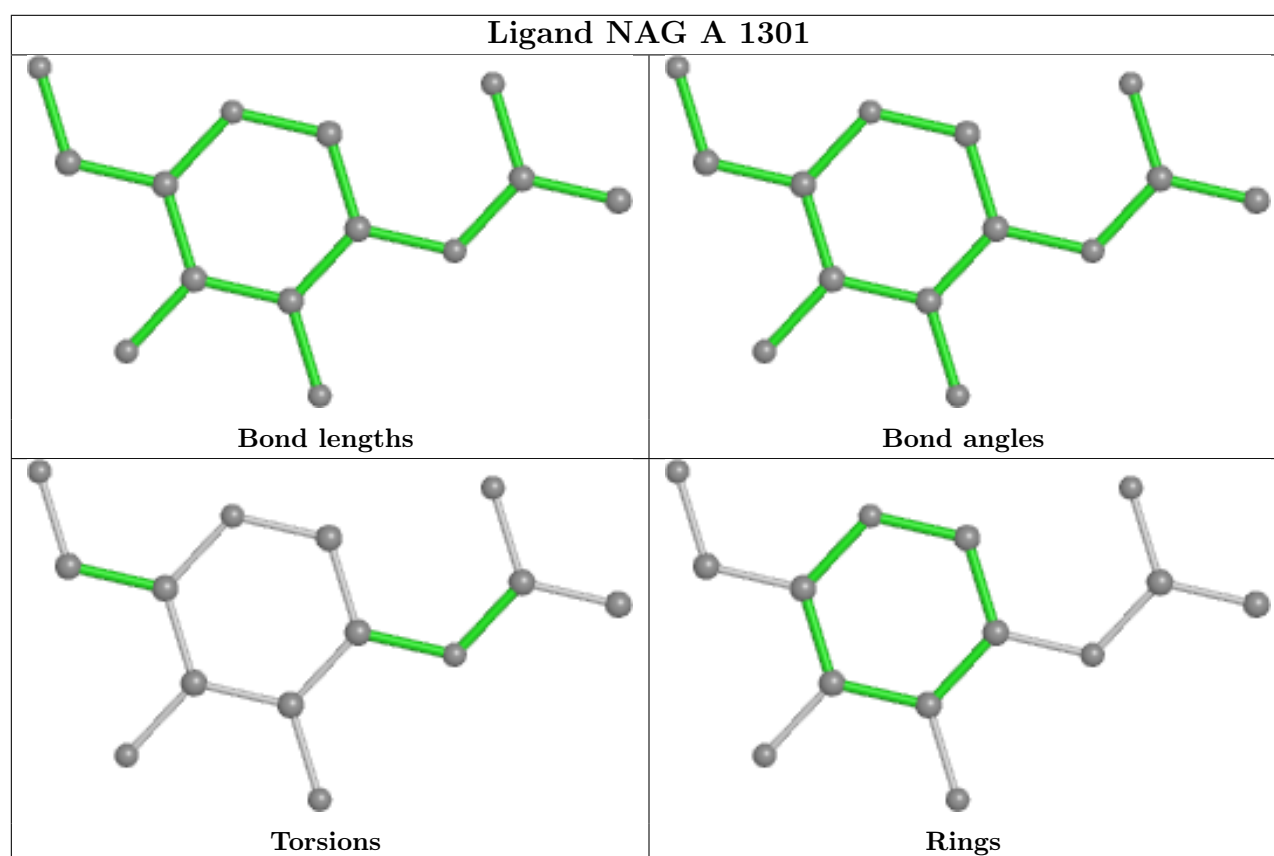
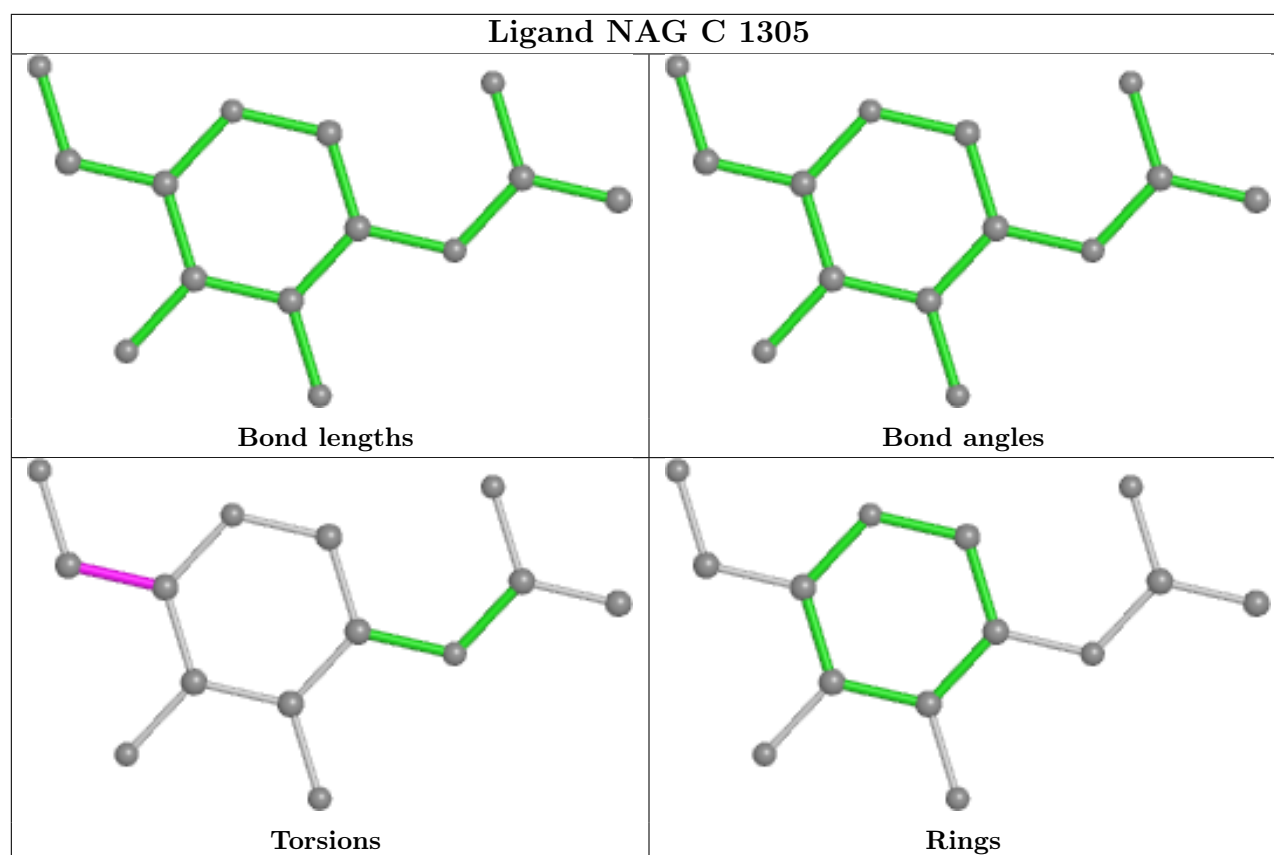
Ligand NAG A 1304

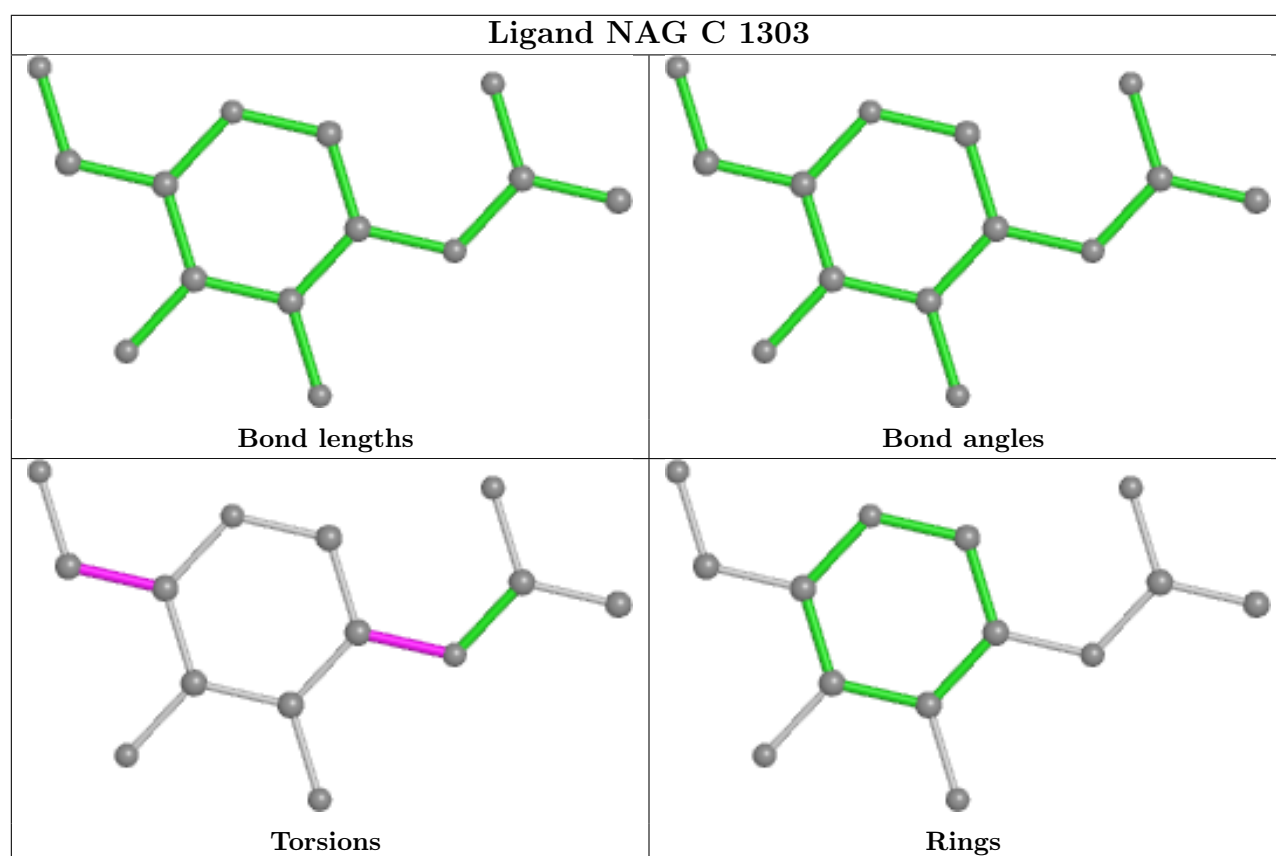
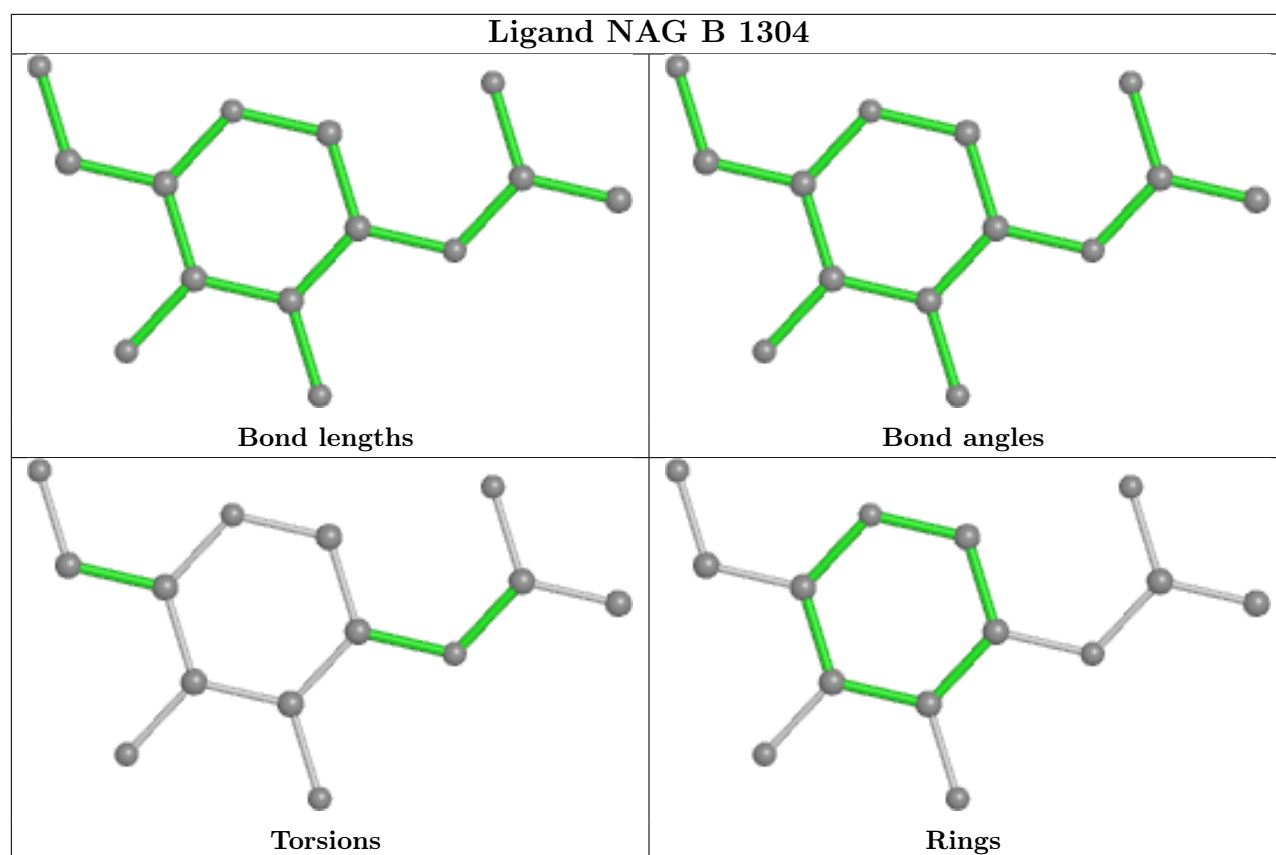


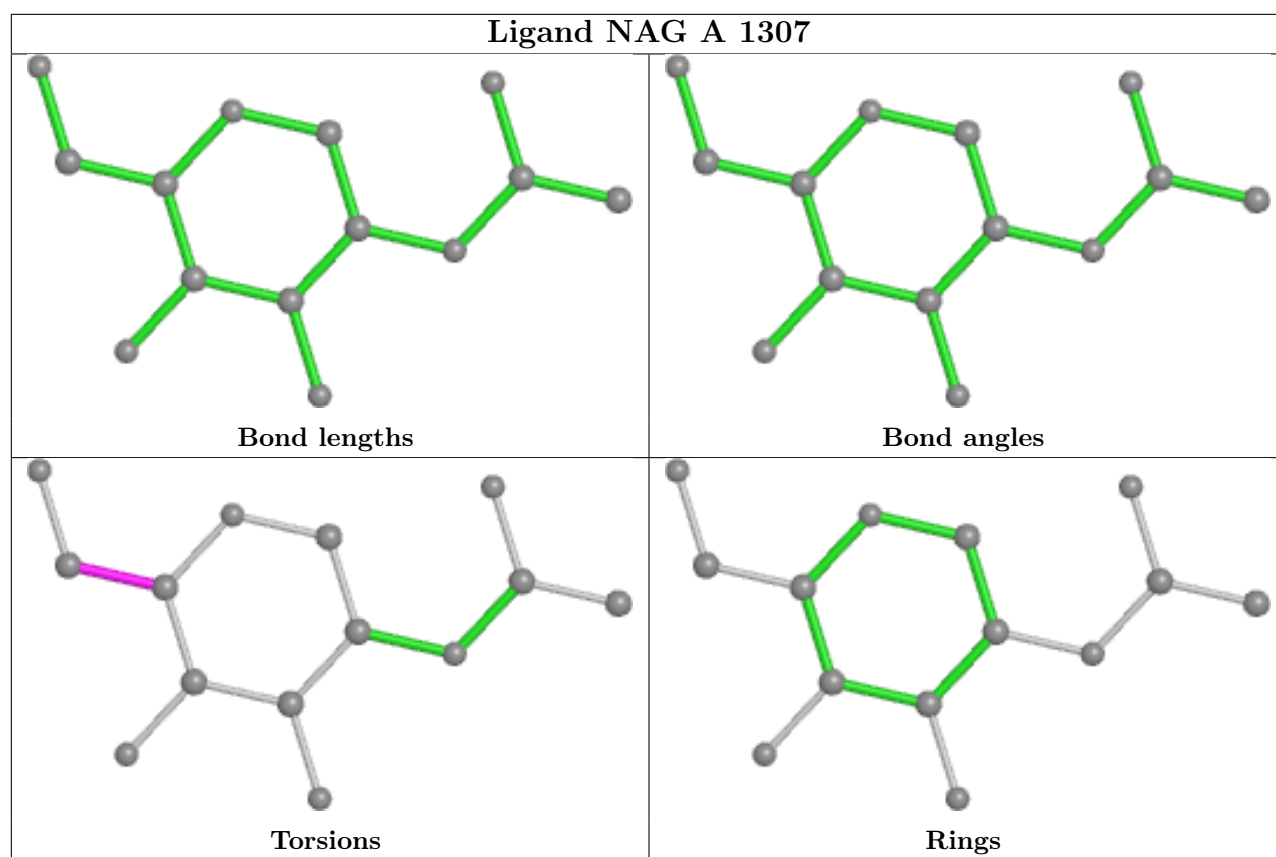












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62734. These allow visual inspection of the internal detail of the map and identification of artifacts.

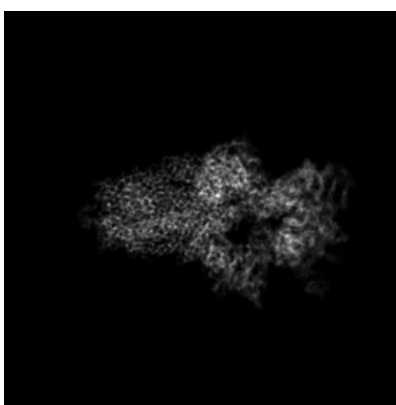
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

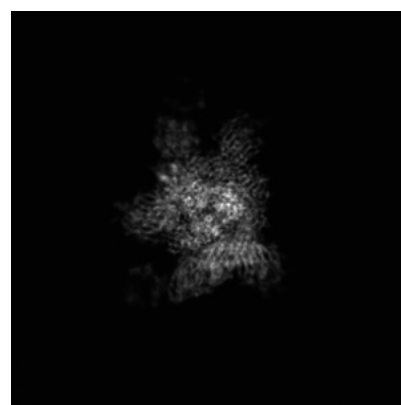
6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 174



Y Index: 164

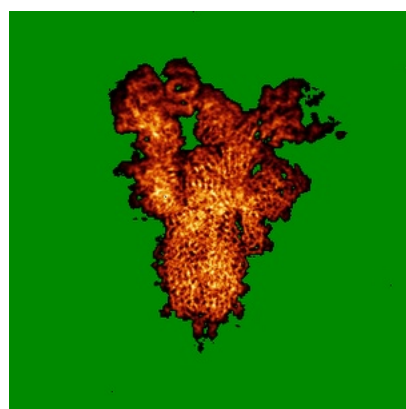


Z Index: 172

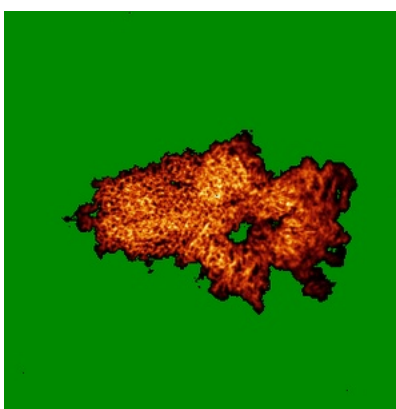
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

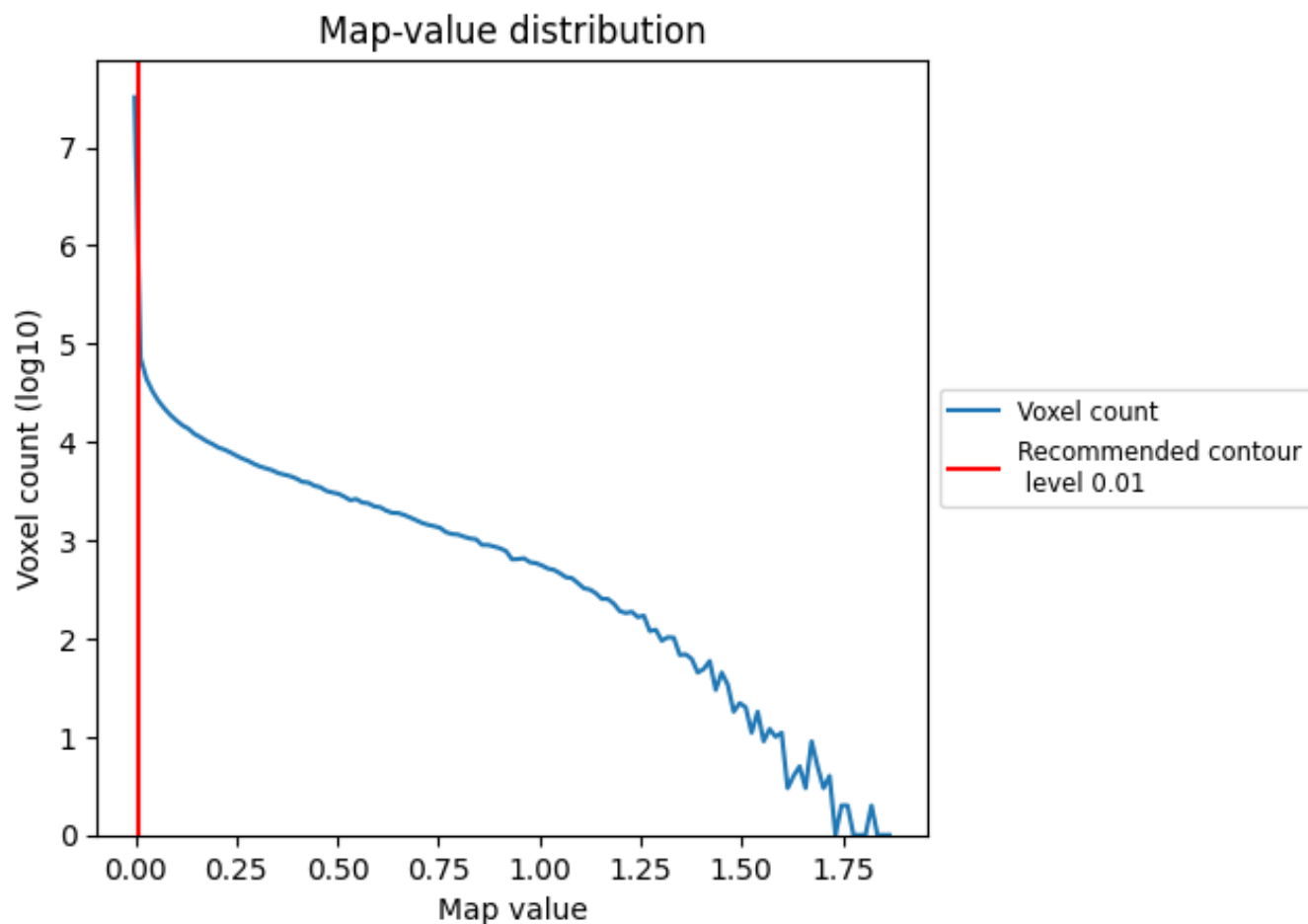
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

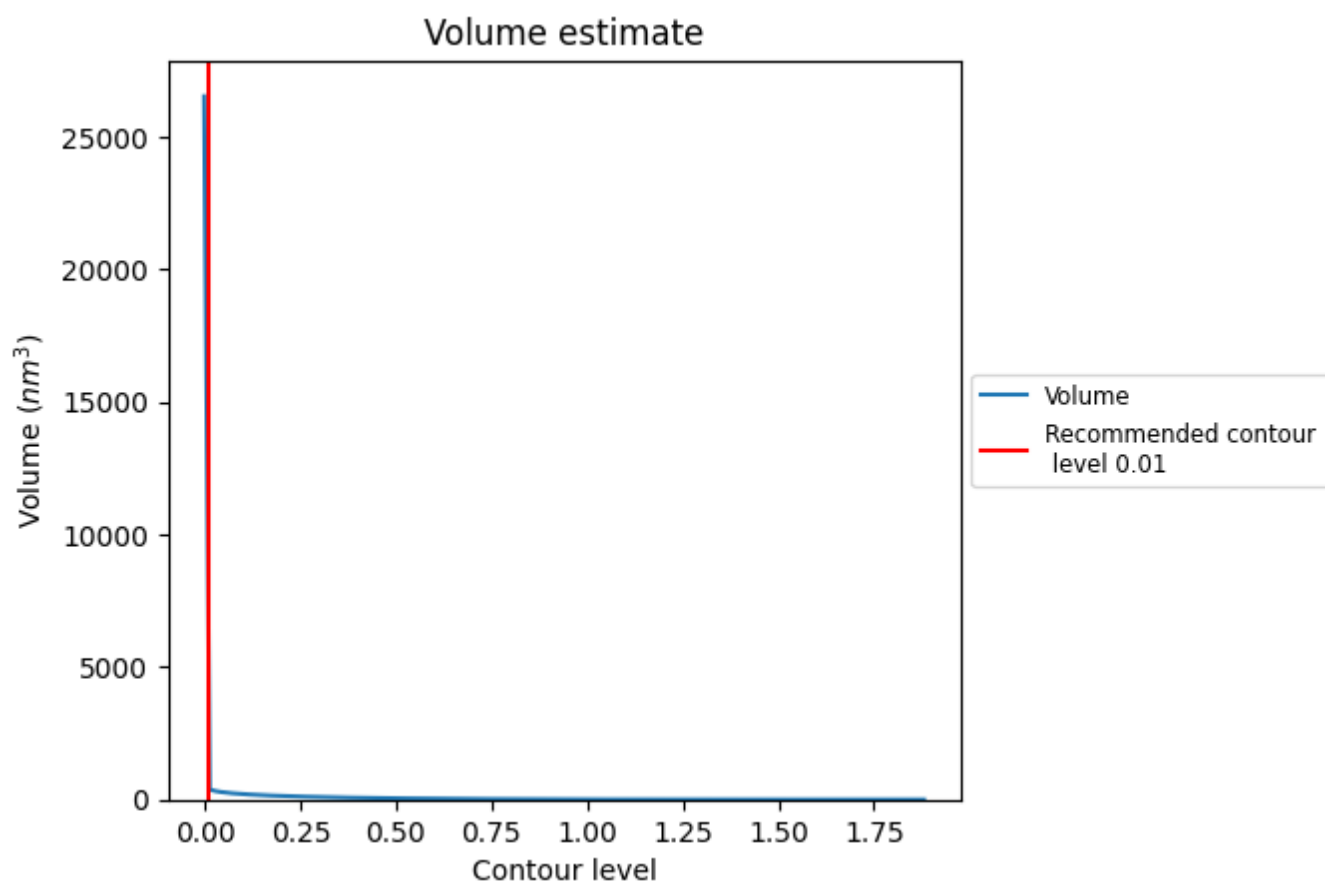
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

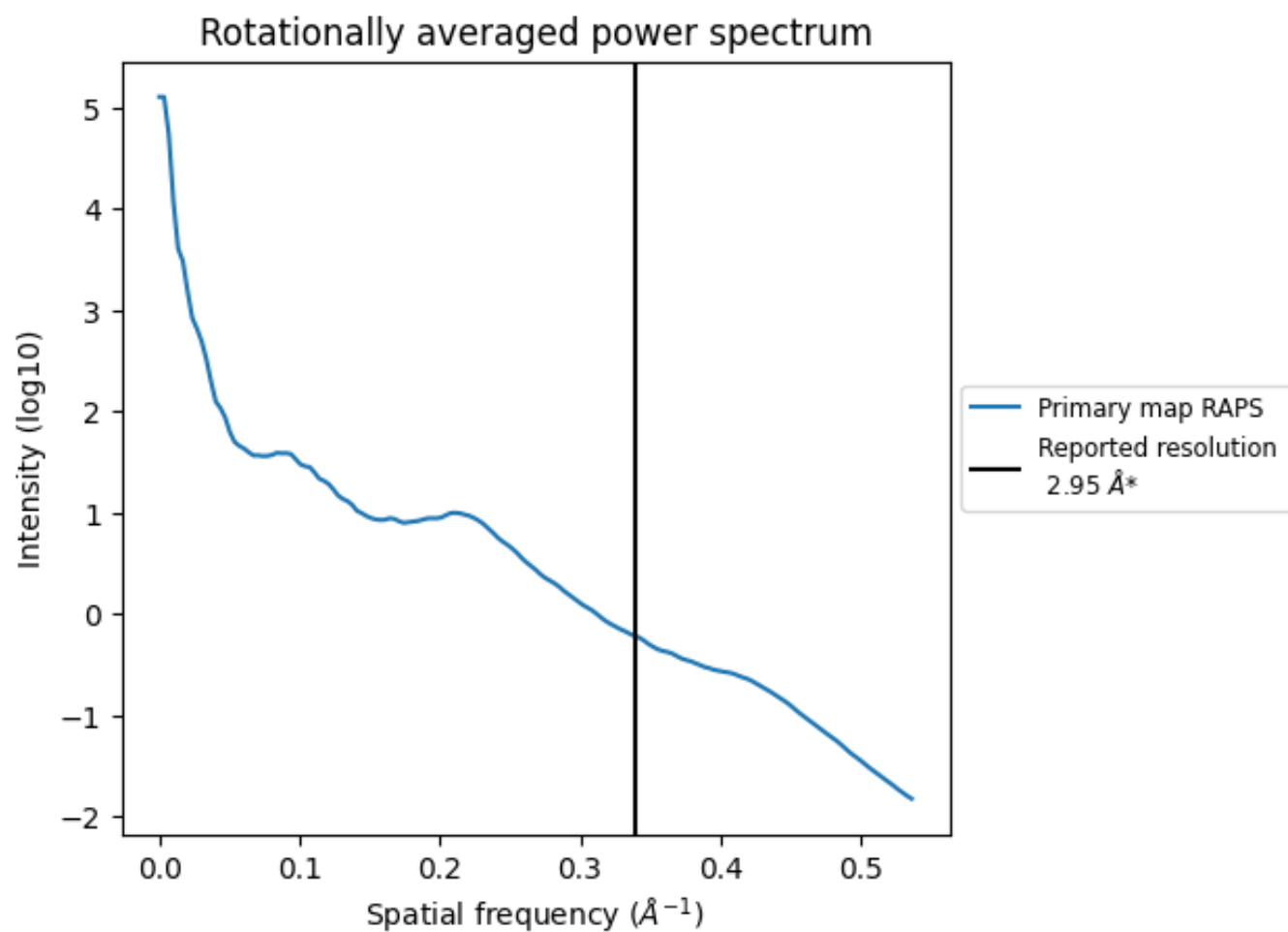
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5627 nm^3 ; this corresponds to an approximate mass of 5083 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.339 Å⁻¹

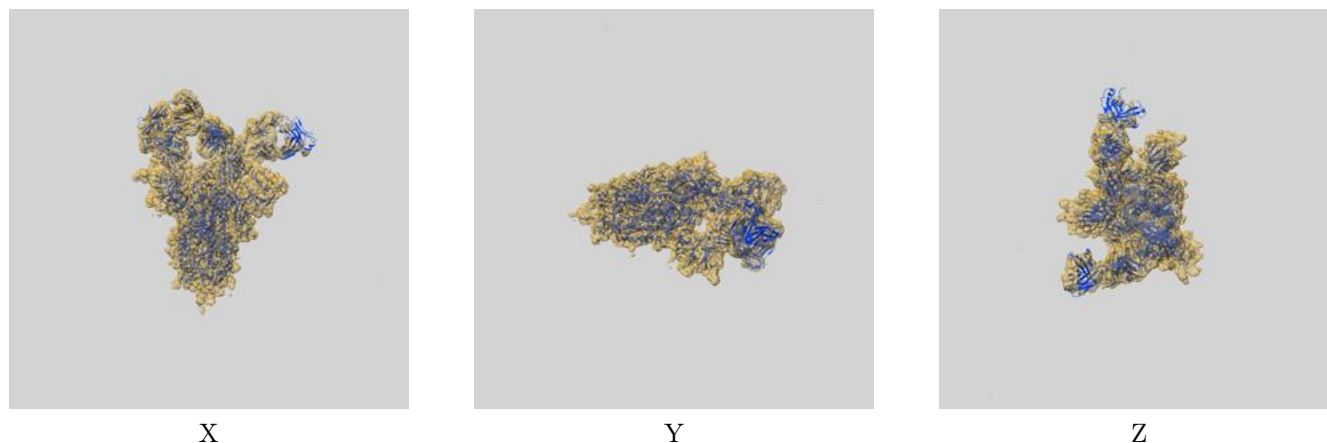
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

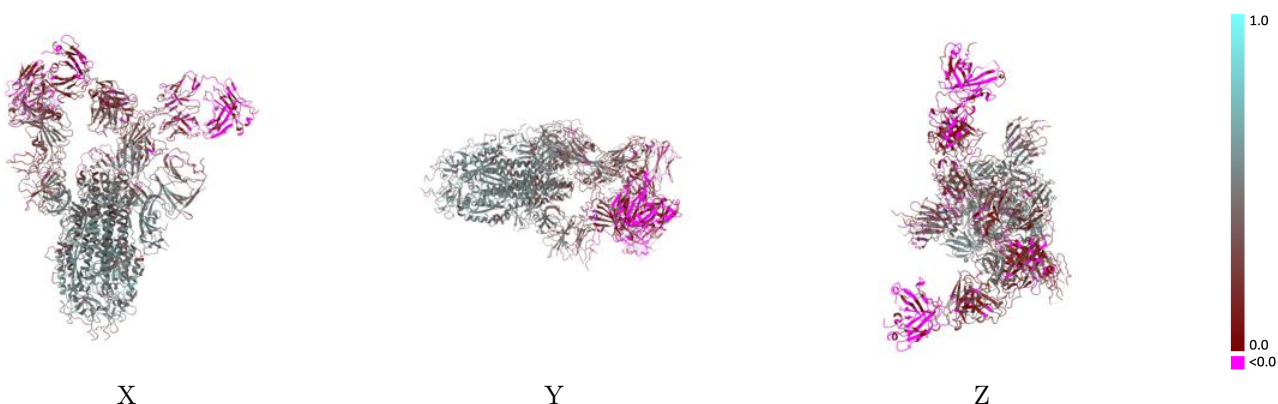
This section contains information regarding the fit between EMDB map EMD-62734 and PDB model 9L15. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



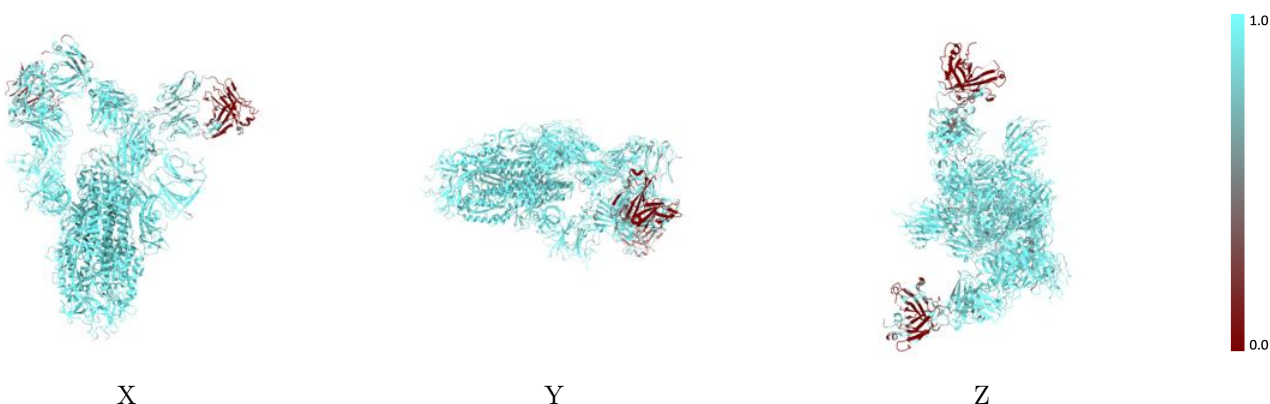
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



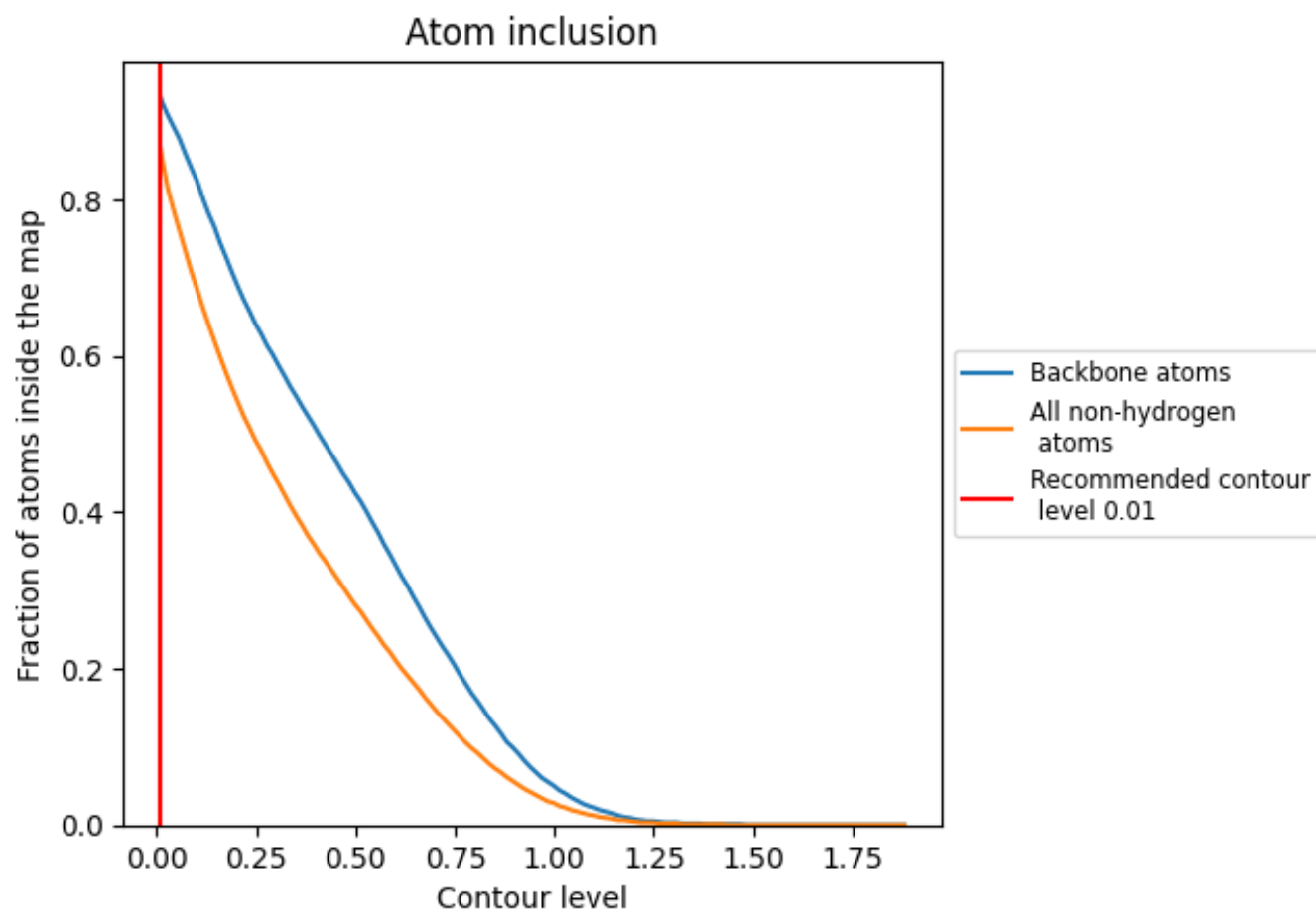
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.3300
A	 0.9420	 0.4280
B	 0.9510	 0.4120
C	 0.9300	 0.4100
D	 0.7140	 0.2250
E	 0.7140	 0.2480
F	 0.7950	 0.1790
G	 0.8570	 0.3960
H	 0.9000	 0.2260
I	 0.6870	 0.1450
J	 0.5840	 0.0590
K	 0.8930	 0.3310
L	 0.8460	 0.1510
M	 0.6210	 0.0890
N	 0.4320	 0.0280
O	 0.8210	 0.3120
P	 0.7860	 0.2910
Q	 0.7860	 0.3430
R	 0.8210	 0.3660
S	 0.9290	 0.3290
T	 0.7140	 0.1980
U	 0.5000	 0.1730
V	 0.8210	 0.3190
W	 0.7140	 0.2160
X	 0.8570	 0.2630
Y	 0.8570	 0.2540
Z	 0.6070	 0.0660
a	 0.7140	 0.1920
b	 0.7860	 0.2810
c	 0.8570	 0.3710
d	 0.7500	 0.2750

